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FUEL MODIFICATION FOR ABATEMENT OF AIRCRAFT TURBINE ENGINE OXIDES OF NITROGEN EMISSIONS

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Esso Research and Engineering Company

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ESSO RESEARCH AND ENGINEERING COMPANY
Government Research Laboratory
Linden, New Jersey

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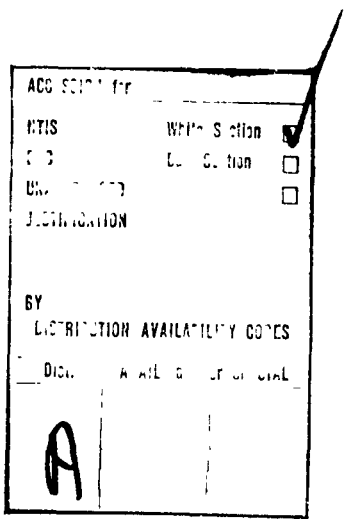

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13. ABSTRACT

This report describes a broad experimental program that was undertaken to assess the feasibility of reducing NO_x from aircraft gas turbine engines by fuel modification. The Esso High Pressure Cannular Combustor was used to simulate the characteristic emissions of gas turbines at full power operation. Over 70 fuel modifications were tested using Jet A as the base fuel.

Soluble compounds of cobalt, iron, magnesium, and copper reduce NO_x by as much as 30% when added to the fuel at a treat rate of up to 0.5% (w). Compounds of sodium reduce NO_x by as much as 26% when added as suspensions or in aqueous emulsions. An aqueous emulsion containing 37 ppm (w) hydrazine acetate reduce NO_x by 15%, but this modification was not consistently effective. None of the investigated additives were fully acceptable because of the relatively low NO_x reduction that was obtained even with high additive treat rates.

A simple expression was derived which is useful in estimating NO levels in gas turbine combustors when equilibrium NO_x concentrations and tempeature are known.

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FOREWORD

This report describes a study carried out by Esso Research and Engineering Company for the United States Air Force under Contract No. F33615-71-C-1575. The study examined the feasibility of reducing oxides of nitrogen emissions from aircraft turbine engines by fuel modification. The work was performed from April 26, 1971 to May 31, 1972 at the Esso Research Center in Linden, New Jersey. Lt. William S. Blazowski of the Air Force Aero Propulsion Laboratory was the responsible Government Engineer. Capt. Donald L. Champagne held this position during the initial phase.

The experimental work was skillfully carried out by Mr. C. J. McCoy. Valuable advice was obtained from Messrs. V. J. Siminski, O. G. Lewis, A. Skopp and Dr. J. P. Longwell.

This technical report has been reviewed and is approved.

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ABSTRACT

A broad experimental program was undertaken to assess the feasibility of reducing NO_x from aircraft gas turbine engines by fuel modifications (additives and/or treatments). The modifications were selected without regard to practical limitations in order not to obscure potentially useful approaches. The Esso High Pressure Cannular Combustor was used to simulate the characteristic emissions of gas turbines. Over 70 fuel modifications were tested using Jet A as the base fuel.

Soluble compounds of cobalt, iron, manganese and copper reduced NO_x by as much as 30% when added to the fuel at a treat rate of up to 0.5% (w) metal. Compounds of sodium reduced NO_x by as much as 26% when added in suspensions or in aqueous emulsions. An aqueous emulsion containing 37 ppm (w) hydrazine acetate reduced NO_x by 15%, but this modification was not consistently effective. None of the investigated additives was fully acceptable because of the relatively low NO_x reduction that was obtained even with high additive treat rates.

The experimental work was carried out at an overall air to fuel ratio of around 50 and at a pressure of 48 psig. The exhaust gas composition was representative of aircraft turbine engines with the exception of the carbon monoxide levels which were too high. A statistical analysis of results with unmodified Jet A fuel indicated that variation of air inlet moisture from 0.00025 to 0.0025 lb of water per lb of air, and pressure variations between 45 and 60 psig had an insignificant effect on NO_x production over the range of the experimental work.

A simple expression was derived which is useful in estimating NO_x levels in gas turbine combustors when equilibrium NO concentrations and temperatures are known.

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SECTION I

SUMMARY

A broad experimental program was undertaken to assess the feasibility of reducing NO_x from aircraft gas turbine engines by fuel modifications (additives and/or treatments). The modifications were selected without regard to practical limitations in order to fully evaluate the fuel modification concept and to uncover promising leads. Practical considerations could obscure potentially useful approaches.

The Esso High Pressure Cannular Combustor was used to simulate the characteristic emissions of gas turbines. Approximately 70 fuel modifications were tested using Jet A as the base fuel. These fell into seven general categories:

(1) Soluble organometallic additives which become heterogeneous reduction or decomposition catalysts.

(2) Additives that scavenge or recombine oxygen atoms.

(3) Additives that reduce peak temperatures.

(4) Additives that delay ignition.

(5) Additives that change spray fluid-dynamics.

(6) Additives that decompose NO or inhibit the NO producing chain reactions.

(7) Combinations of the above for synergistic effects.

Category 1 proved to be the most effective in reducing NO_x emissions. The transition metals added to the Jet A fuel as organometallic compounds reduced NO_x more effectively than other additives. In particular, compounds of cobalt, iron, manganese and copper reduced NO_x by as much as 30% when added to the fuel at a treat rate of up to 0.5% (w) metal. In the alkali metal family, sodium proved most effective by reducing NO_x up to 26% at a treat rate of 0.1% (w). Sodium was added in a suspension as a carbonate or in an aqueous emulsion as a hydroxide. Zirconium reduced NO_x by 11% and 22% at treat rates of 0.1 and 0.2% (w) metal respectively. An aqueous emulsion containing 37 ppm (w) hydrazine acetate reduced NO_x by up to 15%, but this modification gave erratic results.

Most other additives were either ineffective or reduced NO_x by less than 10%. It is noteworthy that all nitrogen containing compounds added at treat levels of more than 0.5% (w) increased NO_x by about 50%. This corresponds to a conversion of up to 30% of the chemically bound nitrogen to NO_x. None of the investigated additives was fully acceptable because of the relatively low NO_x reduction that was obtained even with nigh additive treat rates.

The experimental work was carried out at an overall air to fuel ratio of around 50 and at a pressure of 48 psig. The exhaust gas composition was typical of the latest aircraft turbine engines with the exception of the carbon monoxide levels which were too high. A statistical analysis of results with unmodified Jet A fuel indicated that variation of air inlet moisture from 0.00025 to 0.0025 lb of water per lb of air, and pressure variations between 45 and 60 psig had an insignifcant effect on NO_x production over the range of the experimental work.

A kinetic analysis of the mechanism for NO formation at elevated temperature due to air fixation indicated that the experimental results are reasonable. A simple expression was derived which is useful in estimating NO_x levels in gas turbine combustors when the equilibrium NO concentration and temperature are known.

SECTION II

INTRODUCTION

The oxides of nitrogen (NO_x) are one of the major air pollutants in our atmosphere. On a total tonnage basis, the combustion of fossil fuels in motor vehicles, electric power plants, and industrial boilers accounts for most of the emissions of NO_x. However, the relative importance of uncontrolled NO_x emissions from various smaller sources such as jet aircraft can be expected to increase in the future as increasingly stringent air pollution controls take effect for automobiles and stationary combustion equipment. Consequently, the NO_x problem associated with such sources as jet aircraft can no longer be ignored in the overall national effort to improve the quality of our environment.

There are two ways in which the problem of controlling NO_x emissions from jet engines can be approached. The first would be to modify the engine design, primarily the combustor section, in order to provide temperature, residence time and oxygen concentrations less favorable to the formation of nitrogen oxides. Unfortunately, such engine modifications would cost billions of dollars and take years to fully implement. The alternate approach involves modifying the fuel to reduce NO emissions. Compared to engine modifications, the potential savings in both cost and time that the fuels approach provides is simply too great to dismiss without some kind of broadly based systematic empirical study.

1. NO_x FORMATION

Oxides of nitrogen (NO_x) are produced in all fuel combustion processes using air as the oxidizer. At flame temperatures, the combination of atmospheric oxygen and nitrogen results in the formation of nitric oxide (NO). The rate of NO formation and decomposition is very highly temperature-dependent. The mechanism of formation of NO from nitrogen and oxygen follows the chain reaction sequence first postulated by Zeldovich (1) for the H_2-O_2-N_2 reaction system and confirmed by shock tube studies on N_2-O_2 mixtures (2).

$$O_2 + M \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2O + M \qquad (1)$$

$$O + N_2 \underset{k_4}{\overset{k_3}{\rightleftharpoons}} NO + N \qquad (2)$$

$$N + O_2 \underset{k_6}{\overset{k_5}{\rightleftharpoons}} NO + O \qquad (3)$$

Although it is now generally accepted that the bulk of the NO in combustion processes is produced by the Zeldovich mechanism, recent studies (3), with premixed flat flames indicate that NO may be formed at rates higher than this mechanism predicts for hydrocarbon/air combustion. This "prompt NO" formation, which has not been observed in either hydrogen/air flames or CO/air flames may involve an attack of carbon or hydrocarbon radical on nitrogen molecules. This could result in the formation of HCN and atomic nitrogen which would then lead to the formation of NO at rates higher than those predicted by the Zeldovich mechanism. On the other hand, the reported high rates of NO might be equally well explained by the existence of super-equilibrium concentrations of O-atoms in the flame zone.

Besides the atomic chain route, NO can also be formed by reaction (4).

$$OH + N \underset{k_8}{\overset{k_7}{\rightleftharpoons}} NO + H \qquad (4)$$

This reaction becomes important only under fuel rich conditions where the low oxygen concentration decreases the rate of reaction (3).

The kinetic mechanism consisting of reactions (1) through (4) can be solved analytically by assuming that all combustion is complete prior to NO formation, all combustion species except NO are in chemical equilibrium at the adiabatic flame temperature, and nitrogen atoms have achieved a steady state ($d(N)/dt = 0$). A full mathematical treatment is given in Appendix VI. The resulting expression is:

$$(\delta + 1) \ln (1-\rho) + (\delta-1) \ln (1 + \rho) = -\theta t \qquad (5)$$

where,

$$\delta = \frac{\frac{k_4}{k_5} K_{NO}^{\frac{1}{2}} \left(\frac{X_{N_2}}{X_{O_2}}\right)^{\frac{1}{2}}}{1 + \frac{k_7}{k_5}\left(\frac{X_{OH}}{X_{O_2}}\right)}$$

ρ = reduced NO mole fraction with respect to equilibrium = $\frac{X_{NO}}{X_{NO,e}}$.

t = time in seconds.

X_i = mole fraction of component i.

P = pressure in atmospheres.

R = gas constant = $82.057 \frac{cm^3\ atm}{mole\ ^\circ K} = 1.987 \frac{cal}{mole\ ^\circ K}$.

T = temperature in $^\circ K$.

$$\theta = \frac{4k_3 K_o^{\frac{1}{2}} P^{\frac{1}{2}} X_{N_2}^{\frac{1}{2}}}{K_{NO}^{\frac{1}{2}} RT}, \text{ sec}^{-1}.$$

Equation (5) can be simplified for the practical conditions of aircraft combustion where $\rho \lesssim 0.2$ and $\delta < 0.8$ with an error of less than 9% to

$$\rho = \frac{\theta t}{2}. \qquad (6)$$

Equation (6) is useful for estimating NO levels in gas turbine combustors with fair accuracy since "prompt NO" is minimal under fuel lean conditions. This will be illustrated in Section IV which describes the results.

Organic nitrogen compounds present in the fuel provide another source of NO in combustion processes. Based on experimental evidence, the role of fuel nitrogen appears to vary from being the dominant source of NO at low combustion temperatures to being of minor importance at high temperatures. In general, this source of NO is not important in aircraft engine operation since jet fuel contains less than 50 ppm (w) nitrogen and would contribute less than 0.16 lb NO_x (as NO_2) per 1000 lb of fuel.

The main environmental problem associated with NO_x emissions is actually due to NO_2. The background presented above relating to NO formation is important because NO is the major precursor to NO_2 formation. Nitrogen dioxide contributes to pollution by reacting with hydrocarbons, ozone and light to produce smog. In addition, NO_2 reacts with water to produce acid which causes corrosion problems, and it absorbs visible light which reduces visibility as well as contrast and brightness of distant objects.

From the standpoint of minimizing total NO_x emissions, it is fortunate that the concentration of NO_2 in and near the combustion zone is very low. This results from the fact that NO_2 is thermodynamically unfavorable at combustion temperatures. In addition to this thermodynamic limitation, there is also a kinetic limitation at high temperature. The oxidation of NO by O_2 via reaction (7) is one of the few known reactions

$$2NO + O_2 \longrightarrow 2NO_2 \qquad (7)$$

whose reaction rate decreases with increasing temperature (4). The consequence of these thermodynamic and kinetic limitations is that the amount of NO_2 emitted by combustion sources is limited to a few percent and only as the combustion gases cool in the atmosphere does any significant amount of the reddish brown NO_2 begin to form. The other six oxides of nitrogen (N_2O, N_2O_2, N_2O_3, N_2O_4, N_2O_5, NO_3) play only insignificant roles in combustion processes.

2. AIRCRAFT GAS TURBINES

In an aviation gas turbine engine, inlet air is continuously compressed, mixed with liquid fuel, and then burned in a continuous combustor. Quantities of air greatly in excess of the stoichiometric fuel requirement are compressed and used to keep the combustor liner cool and to dilute the combustor exit gases so as to avoid damage to the turbine and nozzle.

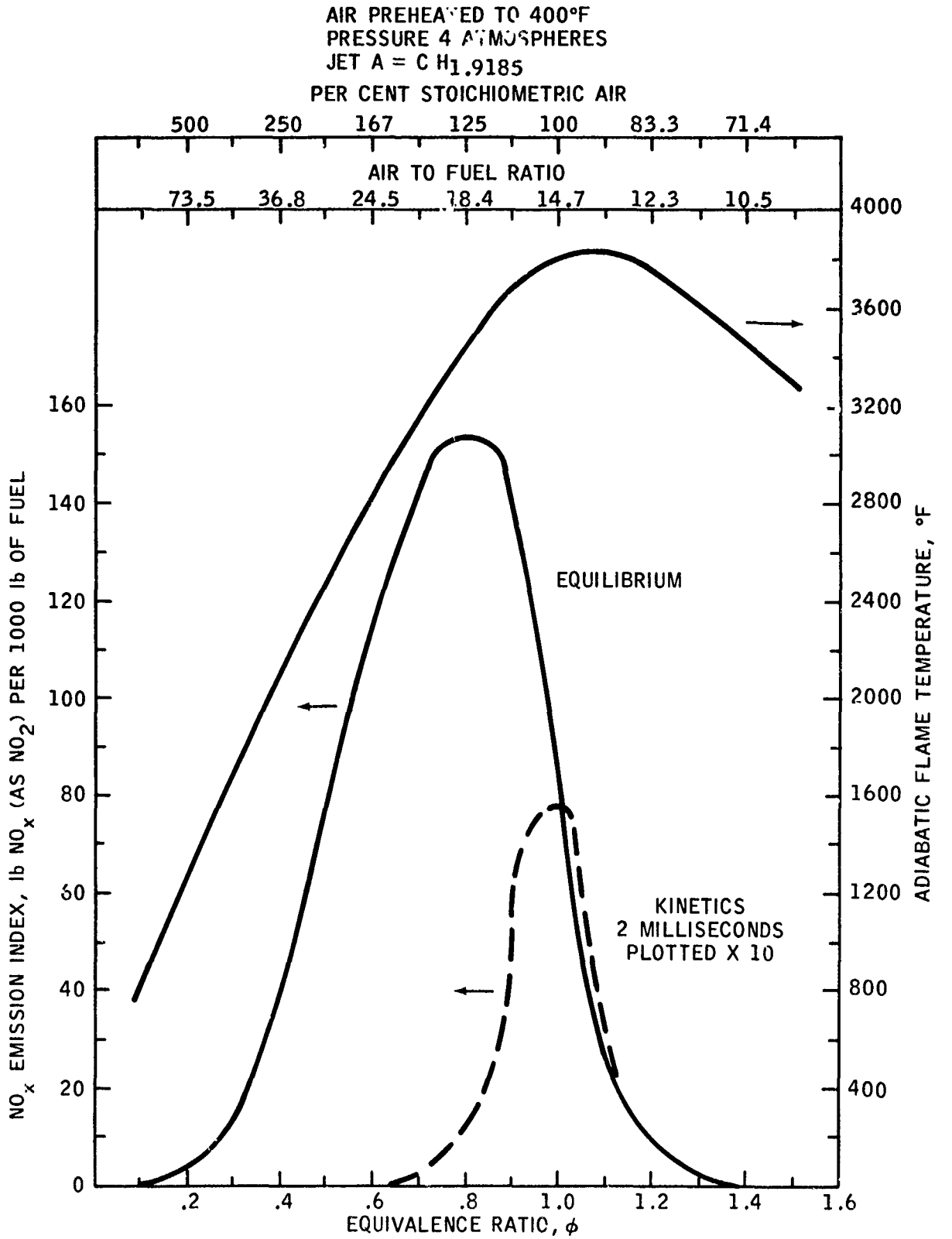

Figure 1

NO_x EQUILIBRIUM IN JET A COMBUSTION

The primary section of the combustor is operated near stoichiometric conditions (generally rich for military operations) and produces combustor gas temperatures in excess of 3800°F depending on the engine pressure ratio. Further down the combustor, secondary air is added which raises the Air/Fuel ratio and lowers gas temperatures. Gas temperatures exiting from the combustor are in the range of 2000°F depending on the engine pressure ratio. The fuel injection pressure varies. It is typically 600 psi for full power and as low as 60 to 100 psi for idle conditions in conventional aircraft. Newer fuel injection techniques involve premixing or carburization where the fuel is atomized and vaporized by shearing with the available air flows. In these aircraft, much lower fuel pressures are required. The pressure drop across the length of aircraft turbine engine combustor is generally about 5%. The total absolute operating pressure is in the range of 20 to 300 psi.

Aircraft turbine engines generally operate more efficiently then reciprocating internal combustion engines and therefore do not exhaust high levels of objectionable gaseous emission. The emissions that are classified as pollutants are emitted either during idle when CO and unburned hydrocarbons are maximized or during full power operation or take-off when NO_x and smoke emissions are maximized.

Since NO_x formation is thermodynamically favored by high temperatures, and kinetic studies indicate that the rate of NO formation has a high activation energy (~115 kcal/mole), the major formation of NO must take place in the high temperature primary combustion zone. This point is illustrated in Figure 1. It is based on computer calculated equilibrium values (5) for the operating conditions used in this experimental program. The kinetic curve was obtained using Equation (6) for 2 milliseconds residence time. The equilibrium and kinetic data were converted into units of emission index in lb per 1000 lb of fuel. This was done in order to present the data in a general format which avoids the effect of dilution. Using emission index, one can rank different aircraft engine designs which may have radically different recirculation patterns as well as other types of power plants. Note that the maximum equilibrium value of NO_x occurs at an equivalence ratio of 0.8 and is a factor of 20 larger than one would calculate based on kinetic limitations. The maximum kinetic value of NO_x is about 7.9 lb/1000 lb of fuel at an equivalence ratio of 1.0. Since gas turbines generally operate at full power at an equivalence ratio of about 0.3, the NO_x produced in the primary zone under stoichiometric conditions is diluted by a factor of about 3.3. By using emission index units, no dilution correction needs to be made.

There have been numerous investigations of the composition of exhaust gases from aircraft gas turbines (6-15). Most of these studies were made with nearly atmospheric pressure cannular combustors or with actual model gas turbines. In general, the exhaust gases from cannular combustors tend to have higher concentrations of carbon monoxide and

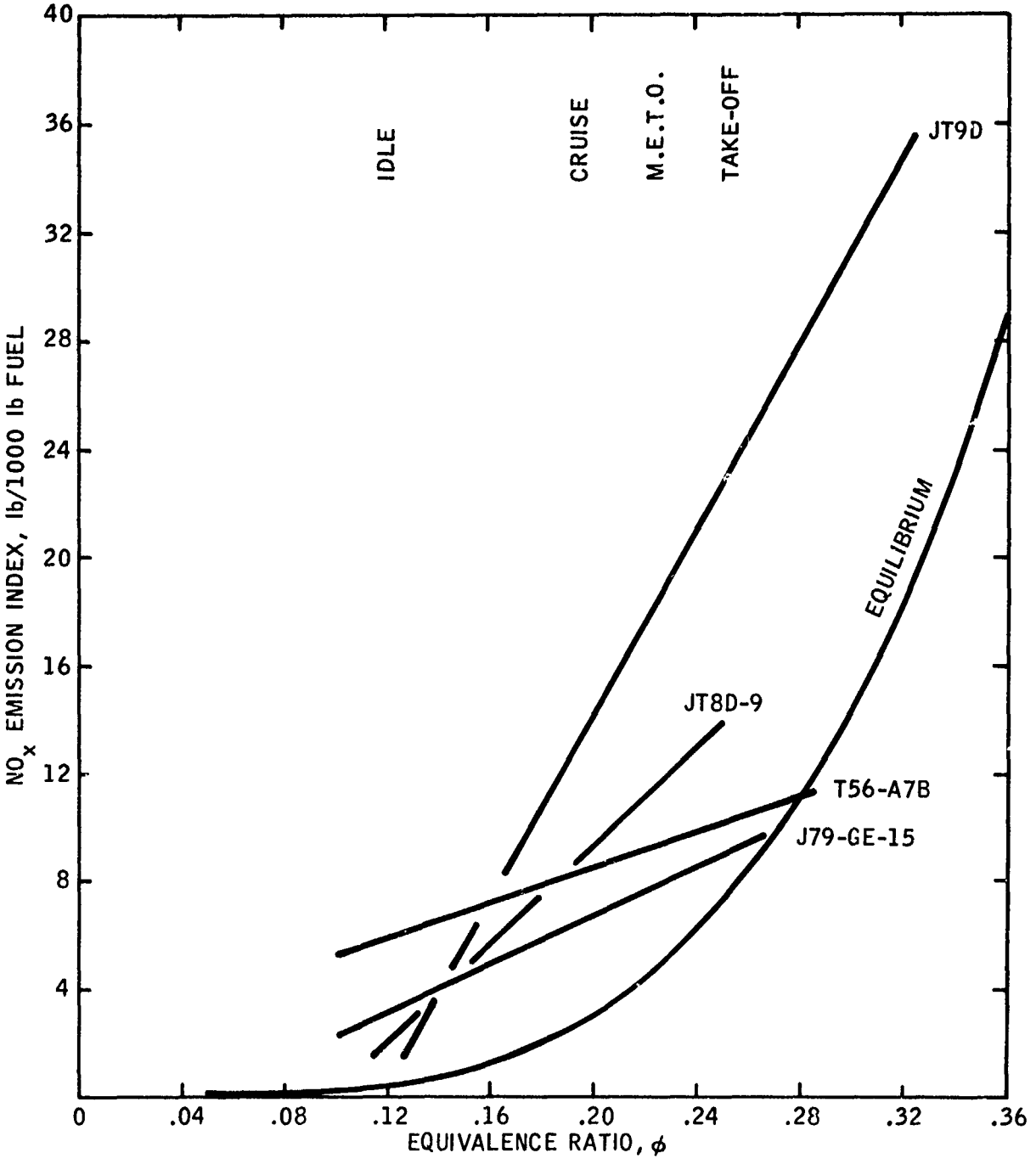

Figure 2

NO_x LEVELS IN AIRCRAFT TURBINE ENGINES

unburned hydrocarbons and lower concentrations of oxides of nitrogen when compared with actual gas turbines. This is partly due to higher surface to volume ratios in laboratory units which make them less adiabatic. Additional factors which cause higher concentrations of CO and unburned hydrocarbons and lower NO_x concentrations in laboratory units are: poorer fuel injection, poorer mixing, less efficient combustion, improper air distribution, and lower air preheat temperatures. In addition to the factors mentioned above, the higher NO_x levels in the exhaust of gas turbines is believed due to higher pressure and temperature operation than in cannular combustors. The concentration of NO which generally comprises in excess of 80% of the NO_x emissions from aircraft gas turbines is not predictable from equilibrium calculations. Figure 2 is a plot of data obtained from emissions measurements from representative aircraft gas turbines (14,15). These experimental results are compared with the equilibrium curve for 4 atm pressure and 400°F preheated air.

Some field surveys of the emissions of aircraft engines were recently published. Cox, Penn and Chase (13) measured the emissions of 25 aircraft turbine engines using Jet A fuel. Their results are presented in Table I. Hare, Dietzmann and Springer (14) reported on emissions measurements from two military engines and six commercial engines. Their data were converted to emission index units using the equations derived in Appendix V. The average baseline NO_x emissions from the military and commercial engines are presented in Table II. A. W. Nelson (15) measured the emission from nine JT3D, nine JT8D and four JT9D engines. He found that the empirical equations listed in Table III predict his results in pounds of NO_x per pound of fuel. Nelson's average experimental values are given in Table IV. NO_x emission levels of up to 420 ppm or an emission index of 36.8 lb per 1000 lb fuel were measured with the JT9D engine.

3. FUEL MODIFICATIONS

Very little work has been reported on the use of additives for reducing NO_x emissions. One of the more comprehensive efforts was reported by Martin, Pershing and Berkau (16). They found that no additive was effective in reducing NO_x in stationary power plant boilers, but iron, manganese and cobalt reduced particulate emissions. Some of the nitrogen containing additives increased NO_x emissions. Altwicker, Fredette and Shen (17) reported that 1.0% (v) cobalt naphthenate reduced NO_x in their laboratory burner set-up by 16%. Meguerian (18) investigated the effect of 29 fuel soluble organometallic compounds at a concentration level of one gram of metal per gallon of fuel. He found that chromium acetylacetonate, cobalt octoate, and nickel naphthenate were "very effective" in reducing NO_x under fuel-rich conditions. Copper naphthenate and cerium octoate were "less effective" and the rest of the additives were not effective. Under fuel-lean conditions, none of the additives

TABLE I

AVERAGE GASEOUS EMISSIONS FROM COMMERCIAL AIRCRAFT ENGINES (13)

Mode	Engine operating parameters			Components, lb/1,000 lb fuel			
	Thrust, lb	Fuel, lb/hr	Fuel-air ratio	CO	NO_x	HC	Aldehydes
JT3D-1 ENGINE (1 ONLY)							
Idle	930	900	0.0078	87.1	2.0	91.4	5.1
Part power (trim)	8,400	4,500	.0114	4.7	8.3	.25	.08
Cruise	8,750	4,690	.0116	4.3	8.4	.27	.06
Maximum continuous	11,610	6,390	.0123	2.3	9.7	.17	.03
Takeoff	14,360	8,170	.0137	1.4	12.5	.11	.02
JT3D-3B ENGINES (3)							
Idle	870	925	0.0075	96.6	2.1	107.9	5.4
Part power (trim)	10,955	5,950	.0114	2.3	9.1	.19	.04
Cruise	10,875	5,895	.0114	2.7	8.6	.20	.05
Maximum continuous	13,280	7,300	.0127	1.7	8.8	.17	.03
Takeoff	15,900	9,185	.0143	1.3	[1]14.2	[1].28	.02
JT8D-1 ENGINES WITHOUT RETROFIT (3)							
Idle	950	1,030	0.0028	45.5	5.1	9.3	1.7
Part power (trim)	9,240	5,410	.0086	3.5	12.0	.16	.03
Cruise	10,650	6,260	.0100	2.7	12.5	.12	.02
Maximum continuous	11,690	6,905	.0105	2.5	14.0	.12	.02
Takeoff	12,545	7,555	.0112	2.5	16.5	.12	.01
JT8D-1 ENGINES WITH RETROFIT (5)							
Idle	995	1,080	0.0041	30.8	2.9	5.5	1.1
Part power (trim)	9,185	5,445	.0100	1.9	11.6	.10	.03
Cruise	10,540	6,260	.0109	1.5	13.4	.11	.03
Maximum continuous	11,680	7,010	.0116	1.4	17.4	.08	.03
Takeoff	12,450	7,480	.0122	1.3	18.9	.07	.03
JT8D-7 ENGINES WITHOUT RETROFIT (2)							
Idle	1,025	1,075	0.0026	44.2	5.1	10.9	1.7
Part power (trim)[1]	9,750	5,740	.0099	2.9	11.6	.08	.04
Cruise	10,860	6,400	.0106	2.5	12.2	.29	.04
Maximum continuous	12,060	7,170	.0116	2.1	13.8	.17	.05
Takeoff	13,055	7,885	.0126	1.9	15.2	.10	.05
JT8D-7 ENGINES WITH RETROFIT (2)							
Idle	960	1,060	0.0031	26.8	4.0	5.9	-
Part power (trim)	9,755	5,705	.0101	1.6	12.7	.12	-
Cruise	10,855	6,420	.0114	1.4	14.3	.26	-
Maximum continuous	11,875	7,105	.0124	1.3	15.9	.21	-
Takeoff	12,710	7,685	.0132	1.2	17.1	.16	-
JT8D-9 ENGINES WITH RETROFIT (6)							
Idle	980	1,040	0.0038	28.2	4.7	8.4	1.2
Part power (trim)	10,485	6,095	.0115	1.8	14.3	.11	.04
Cruise	10,830	6,310	.0117	1.7	14.1	.19	.05
Maximum continuous	11,895	6,975	.0126	1.5	15.6	.18	.04
Takeoff	13,570	8,200	.0140	1.2	18.1	.18	.04
511-14 SPEY ENGINES (4)							
Idle	625	915	0.0067	97.5	2.0	57.3	5.6
Takeoff	11,140	7,370	.0147	2.3	18.8	.13	.06
Checkpoint 1	10,705	7,005	.0141	2.4	18.1	.11	.05
Checkpoint 2	10,140	6,545	.0135	2.7	18.5	.11	.04
Checkpoint 3	9,575	6,145	.0130	2.8	18.3	.11	.04
Checkpoint 4	7,490	4,685	.0114	3.9	15.6	.12	.04

[1]One engine only.

TABLE II

AVERAGE NO_x EMISSION INDEX FROM MILITARY AND COMMERCIAL AIRCRAFT ENGINES (14)

MODE ENGINE	Number of Tests	75%	100%	Military	Flight Idle	Cruise	M.E.T.O.	Takeoff	Idle	Reverse
T56-A7B Turboprop	13	8.36	10.2	10.2	6.16					
J79-GE-15 Turbojet	4	5.33	7.12	8.29	2.25					
JT8D-9 Turbofan	17					8.30	10.2	12.6	2.27	11.4
JT8D-1 and JT8D-7 Turbofan	5					7.80	9.25	10.5	2.51	10.1
JT4A-H Turbojet	6					7.61	8.70	10.8	2.13	9.91
JT3D-B Turbofan	8					6.02	7.67	9.60	1.61	8.73
JT3C-6 Turbojet	3					6.70	7.10	8.48	1.35	7.17
CJ805 Turbojet	5					7.55	7.98	9.24	1.70	

TABLE III

EMPIRICAL NO_x MODEL

Engine	Equation
JT8D	$NO_x = .0237 + .0171\ EPR - .214 \times 10^{-5}\ Q$
JT3D	$NO_x = -.0098 + .0140\ EPR - .194\ H$
JT9D	$NO_x = -.093 + .0770\ EPR - .263 \times 10^{-3}\ T - .313\ H$

where Q = Heat of Combustion ~18,500 Btu/lb.

EPR = Engine Pressure Ratio

H = Humidity -lb water/lb air.

T = Inlet Temperature °F.

TABLE IV

AVERAGE GASEOUS EMISSIONS FROM COMMERCIAL AIRCRAFT ENGINES (15)

Engine	Mode	Thrust lbs	Fuel Flow lbs/hr	NO_x lbs/ 1000 lbs Fuel	NO_x 1 Sigma Variation
JT3D	Idle	900	1,070	2.25	0.85
	Approach	5,228	3,573	4.87	0.85
	Climb	16,400	8,120	11.92	0.85
	Takeoff	18,000	9,420	13.63	0.85
JT8D	Idle	800	920	1.71	0.78
	Approach	3,555	2,700	5.39	0.78
	Climb	12,600	7,020	15.60	0.78
	Takeoff	14,500	8,400	18.60	0.78
JT9D	Idle	3,550	1,976	3.41	1.9
	Approach	15,009	7,515	11.42	1.9
	Climb	39,650	14,109	30.00	1.9
	Takeoff	45,500	16,641	36.80	1.9

reduced NO_x. These tests were run in a pulse-flame apparatus. McCreath (19) reported that isoamyl nitrate and ditertiary butyl peroxide reduced NO_x by 17 and 10% respectively in diesel engines. The effectiveness of these additives varied with concentration and age of the blend. Hare et. al. (14) added up to 0.1% (v) CI-2 (see pg. 29 for chemical composition) is some of the aircraft engine tests to determine the effect of additives on the level of emissions. No comprehensive analysis of the data was presented but it appears that hydrocarbons and CO increased slightly while NO_x decreased by up to 8%.

In addition to the organometallic additives mentioned above, there has been considerable work in reducing NO_x from gas turbines by additing water or steam to the combustor primary zone. Klapatch and Koblich (20) reported about 80% reduction of NO_x using 0.9 lb of water per lb of fuel (60 ppm (v) were reduced to 12 ppm (v) at 16 MW operation). They also found that the ratio of NO_2 to NO_x increases as more water is added per pound of fuel.

It was clear from the research described above that the efforts in reducing NO_x emissions should be systematized. In an attempt to broadly evaluate the concept of NO_x reduction with fuel modifications the possible techniques were categorized as follows:

1. Soluble additives which become heterogeneous catalysts for:

   A. Reduction

   $$2NO + 2CO \longrightarrow N_2 + 2CO_2$$

   B. Decomposition

   $$2NO \longrightarrow N_2 + O_2$$

   For example: Co, Na, Fe, Ni, Sb, etc.

2. Additives that scavenge or recombine oxygen atoms

   A. Scavenge

   $$O + CF_3 \longrightarrow COF_2 + F$$

   B. Recombine

   $$O + X_2 \longrightarrow OX + X$$

   $$O + OX \longrightarrow O_2 + X$$

   For example: CCl_4, $(CF_3)_2CHOH$

3. Additives that reduce peak temperature

   A. Radiative heat transfer with solids

   For example: Dicyclopentadiene to produce soot, organometallics to produce oxides

   B. Endothermic physical conversion

   For example: Emulsion of water, alcohol, ammonium formate, hydrazine acetate

4. Additives that delay ignition and thus reduce exposure time at peak temperatures

   For example: analine, ether

5. Additives that change spray fluid-dynamics

   For example: polyisobutylene, dissolved polymers

6. Additives that decompose NO

   $$NO + NH \longrightarrow N_2 + OH$$

   For example: analine, ammonium formate, hydrazine acetate

7. Combination of the above approaches for synergistic effects

   For example: Sb + CCl_4, 0.7 Ni + 0.3 Cu (Monel)

These categories are only an attempt to systematize the research and are not meant to imply that a mechanism for NO_x reduction is known. No attempt to determine the actual NO_x reducing mechanism was made in this program.

The following factors were of secondary importance in this program but should be considered in evaluating the effectiveness of practical fuel modifications:

1. The tendency of fuel additives to cause problems (chemical incompatibility, loss of fuel thermal stability, etc.) generally varies with concentration. Experience indicates that any compound that is required in concentrations greater than about 0.25% by volume in real turbine systems will not be practicable.

2. A "fully effective modification" should, by definition, be capable of reducing the NO_x emission index by more than 90% with a reasonable additive concentration.

3. It is improbable that any modification will find wide acceptance if it increases fuel cost by more than 10% (approximately one cent per gallon modified) when in large quantity production. However, if the fuel additive is used on a demand basis such as during take-off, then a high additive cost could be tolerated.

SECTION III

EXPERIMENTAL

A high pressure cannular combustor was developed in order to test whether potential fuel modifications can reduce oxides of nitrogen emissions. The NO_x emissions from actual aircraft turbine engines can be better simulated with the high pressure laboratory unit than with atmospheric pressure units. A continuous sampling and analytical system was developed which overcomes many of the difficulties and inherent errors of batch sampling. This section describes the design and operation of the combustor and the analytical system.

1. COMBUSTOR

The experimental apparatus consists of a high pressure cannular combustor similar to those used in aircraft gas turbine engines. Figure 3 is a scaled drawing of the Esso Cannular Combustor. The combustor's outer sleeve was initially made out of quartz in order to permit continuous viewing of combustion uniformity. Due to frequent breakage of the quartz, the outer sleeve was changed to one made out of Inconel. Periodic checks with a quartz sleeve showed that the two materials gave equivalent results. A 60-deg hollow cone 0.50 gallon per hour nozzle was used to feed Jet A fuel. Air was fed through a distribution box and was then swirled through the fuel feed zone and the secondary and quench zones. Figure 4 is a photograph of the combustor components. The primary zone (surrounding the nozzle) provided additional swirl by injecting air tangentially. The primary zone average velocity was calculated to be 40 ft/sec which is lower than the 80 ft/sec attributed to modern aircraft combustors. The can was made out of Hastelloy X and is 2 in. in diameter and 6 in. long. The hole sizes in the can provide for the following air distribution.

Primary Zone	30.3%
1 L/D	12.2%
2 L/D	15.9%
3 L/D	41.5%

A minor modification in the equipment was made after Run 46. The modification consisted of dimpling the can after standard construction. A photograph of this dimpled can (Can II) is shown in Figure 5. The original type of can (Can I) was modified to avoid the following problems:

1. Flames occassionally shot out through the secondary air holes of the can. It was necessary to avoid this in order to maintain a consistent basis for determining NO_x reduction with modified fuel.

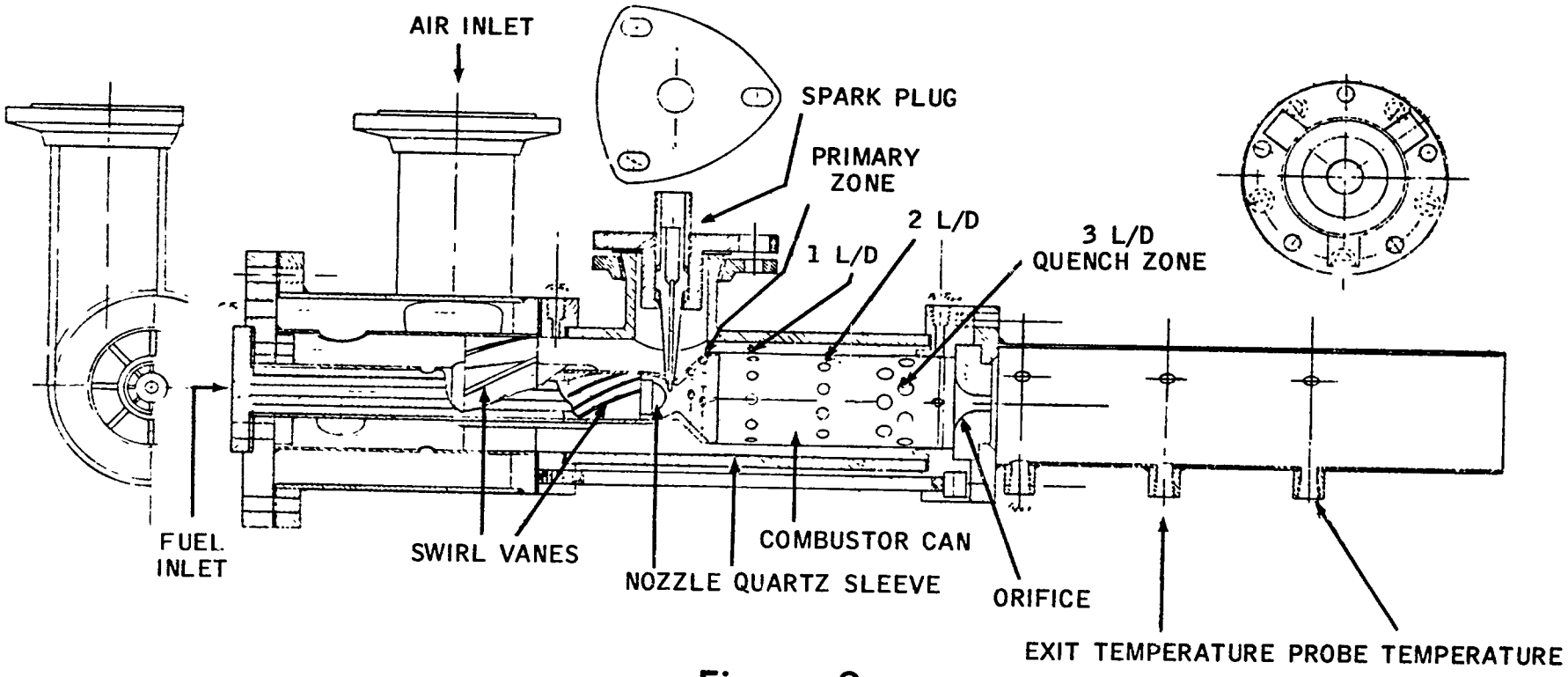

Figure 3

HIGH PRESSURE COMBUSTOR

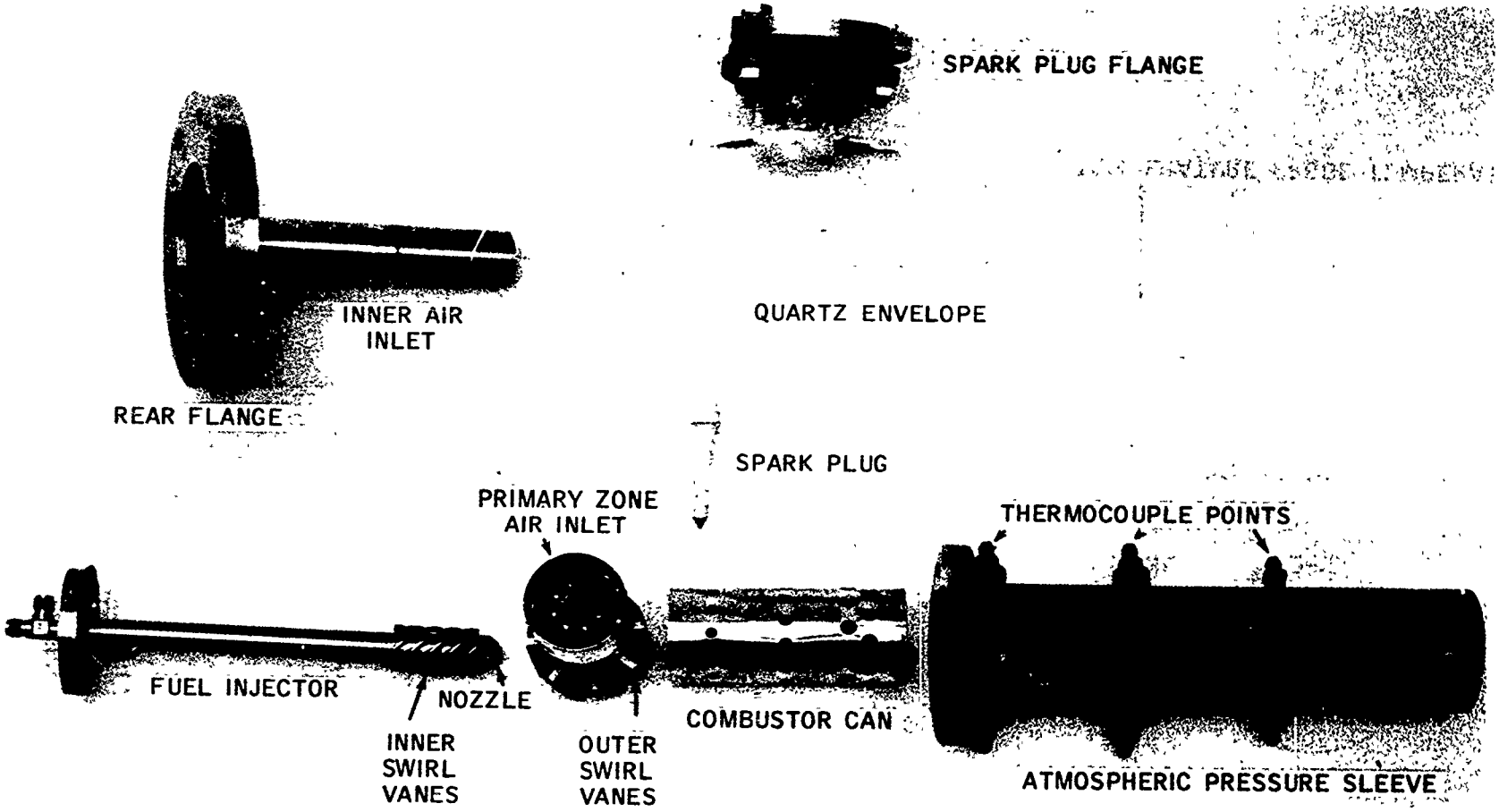

Figure 4
COMPONENTS OF COMBUSTOR

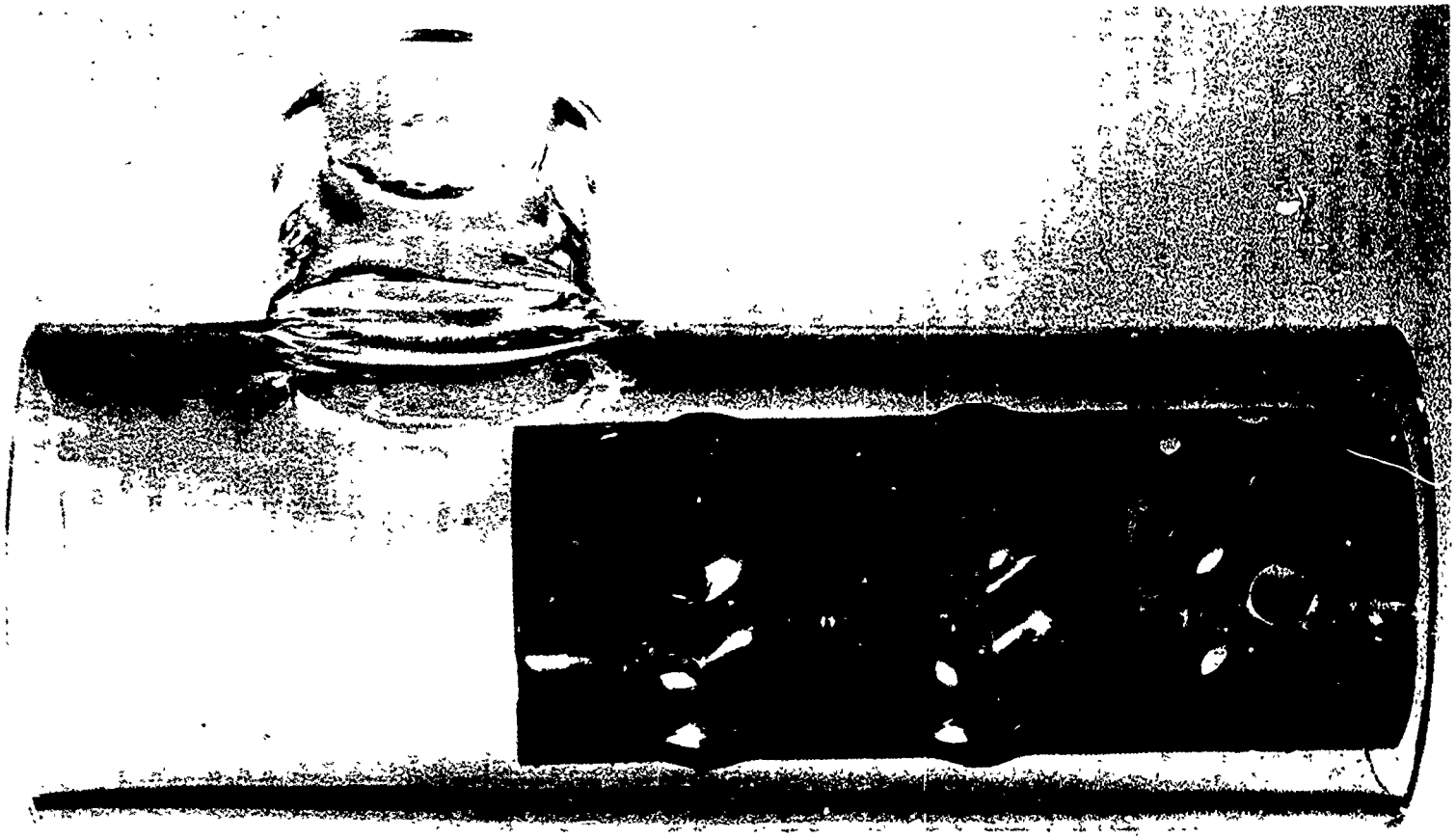

Figure 5
QUARTZ SLEEVE WITH CAN II

2. The can experienced an aging effect after about 20 hours of operation. This caused a decrease in combustion efficiency. The ratio of CO to CO_2 climbed while the NO_x levels and the exit temperatures decreased from expected values. The installation of a new can was necessary in order to continue operation. The reason for the decrease in combustion efficiency was not determined.

One can postulate that the aging problem was caused by ineffective cooling of Can I, thus causing fuel to pyrolyze on the hot metal surface and producing carbon deposits. These deposits further reduced the heat transfer characteristics of the can and provided a hot carbon surface that could reduce NO. The hot carbon surface could also react with the excess oxygen available in the combustor and increase the level of CO. Ultimately the can would fail structurally. An aging effect was recently discussed by H. T. McAdams (21) for JT8D engines. He reported that in 18 tests of engines that had gone up to 3000 hours between overhauls of the hot section, the NO_x levels decreased as engine age increased. McAdams did not discuss the mechanism of NO_x reduction as a function of hot section age.

A high frequency discharge was used for ignition. The combustion gases passed through a stainless steel type 446 orifice which choked the flow to maintain the chamber pressure at 4 atmospheres. The chamber pressure could be increased to 6 atmospheres by changing the orifice plate or by increasing air and fuel flow rates. Static pressure was monitored at three points along the combustor length. The exhaust gases were sampled in a 10" atmospheric pressure sleeve after the orifice. Two sets of chromel-alumel thermocouples 3 in. apart were used to ascertain whether combustion had ceased. One set was located 4.5 in. from the orifice plate and the other set was 7.5 in. from the plate.

2. AIR AND FUEL FEED SYSTEM

The air and fuel feed system is shown schematically in Figure 6. The air feed system consisted of a compressor followed by an 18 ft. diameter sphere. The pressure in the sphere was maintained at approximately 100 psig. The sphere acted as a ballast for maintaining a constant pressure supply of air. The air coming from the sphere was filtered and regulated to 80 psig. The moisture level of the incoming air was continuously monitored. The moisture level varied by a factor of 10 depending on the ambient humidity. After the air flow rate was determined with a rotometer, it was preheated to 425°F.

The fuel feed system consisted of 2 pyrex 5 gallon reservoirs and an Eastern close coupled pump. As can be seen from Figure 6, the pump was used to fill the pyrex vessels as well as to feed fuel to the combustor. A back pressure regulator provided a fuel stream of approximately 350 psig to the fuel feed line while the rest of the fuel was recirculated. The

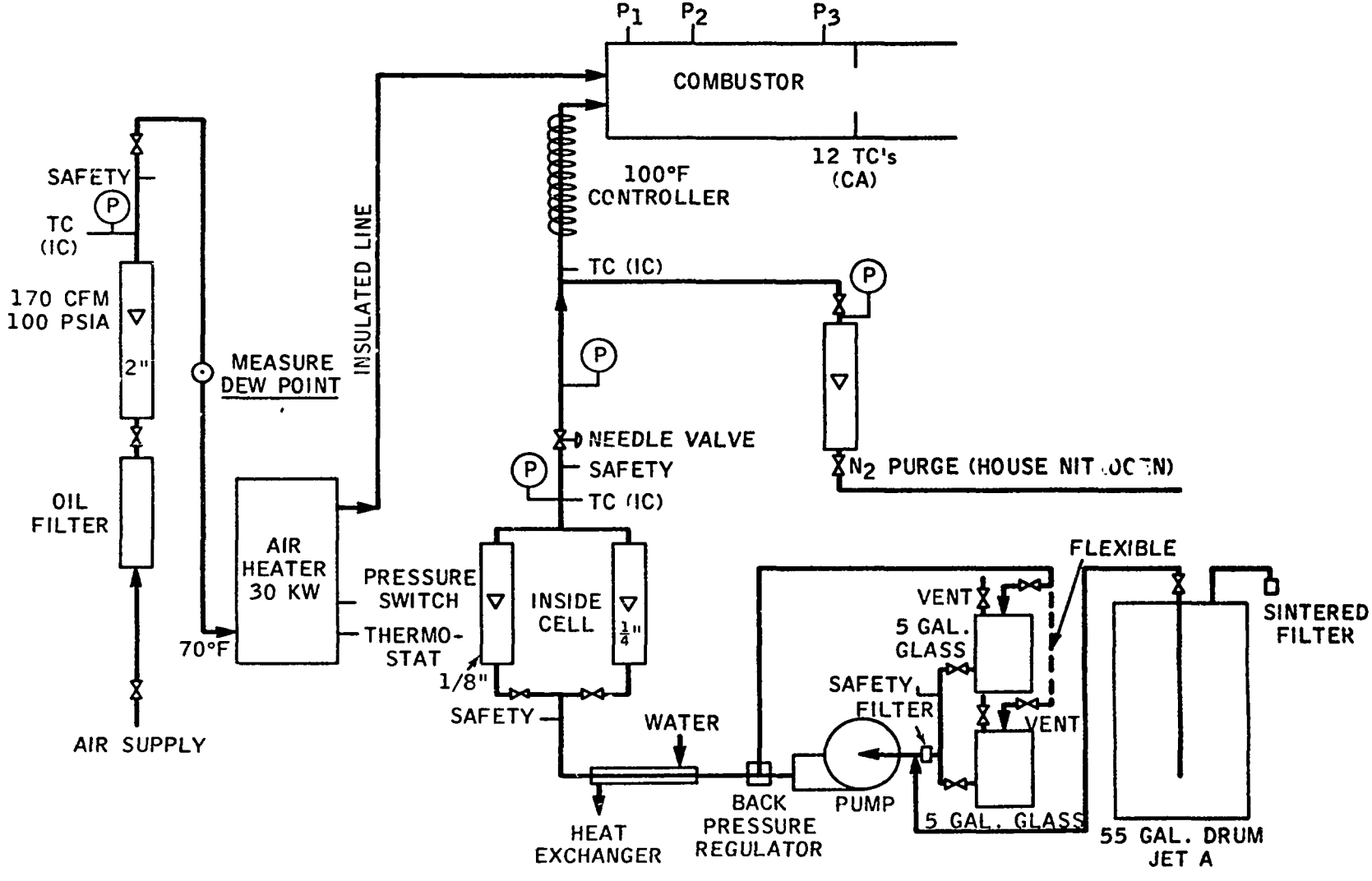

Figure 6

COMBUSTOR FLOWSHEET

recirculation ratio was approximately 10:1. The exact fuel rate was set with a needle valve following a rotometer. One of the reservoir vessels acted as a standard and was never contaminated with additives. The other vessel was used to feed all modified fuels. Since temperature can have a significant effect on the spray dynamics through the nozzle, the fuel was heated to 110°F just prior to injection.

The experimental conditions used throughout this program are listed in Table V. The air flow rate was maintained approximately constant while the fuel was varied for different equivalence ratios. In this manner, the combustor pressure was made independent of equivalence ratio.

TABLE V

EXPERIMENTAL CONDITIONS

Average Air Flow Rate = 162 lbs/hr

Nozzle = 0.5 GPH, 60° Hollow Cone

Orifice Diameter = 0.281 in

Combustor Pressure = 49.2 PSIG

Axial Pressure Drop in Combustor < 0.5 PSIG

Air Preheat = 425°F

Inlet Air Moisture = 400 to 4000 PPM (V)

Fuel Preheat = 110 $\pm$ 5°F

Average Fuel Flow Rate = 3.4 lbs/hr

3. SAMPLING AND ANALYTICAL SYSTEM

The sampling system was designed and constructed to insure that representative samples were delivered to the various instruments. Tests indicated that the total analytical and sampling system provided a rapid response to changes in the emission levels in the combustor effluent. Details of the sampling system are shown in Figure 7. The sample gases from the quartz probe passed through a heated sample line. Quartz probes were used in order to avoid catalytic reduction of NO by CO (22). Exhaust gases flowed through a Teflon tube which was contained in a larger metal tube wrapped with heater tapes. A Gardsman Temperature controller was used to

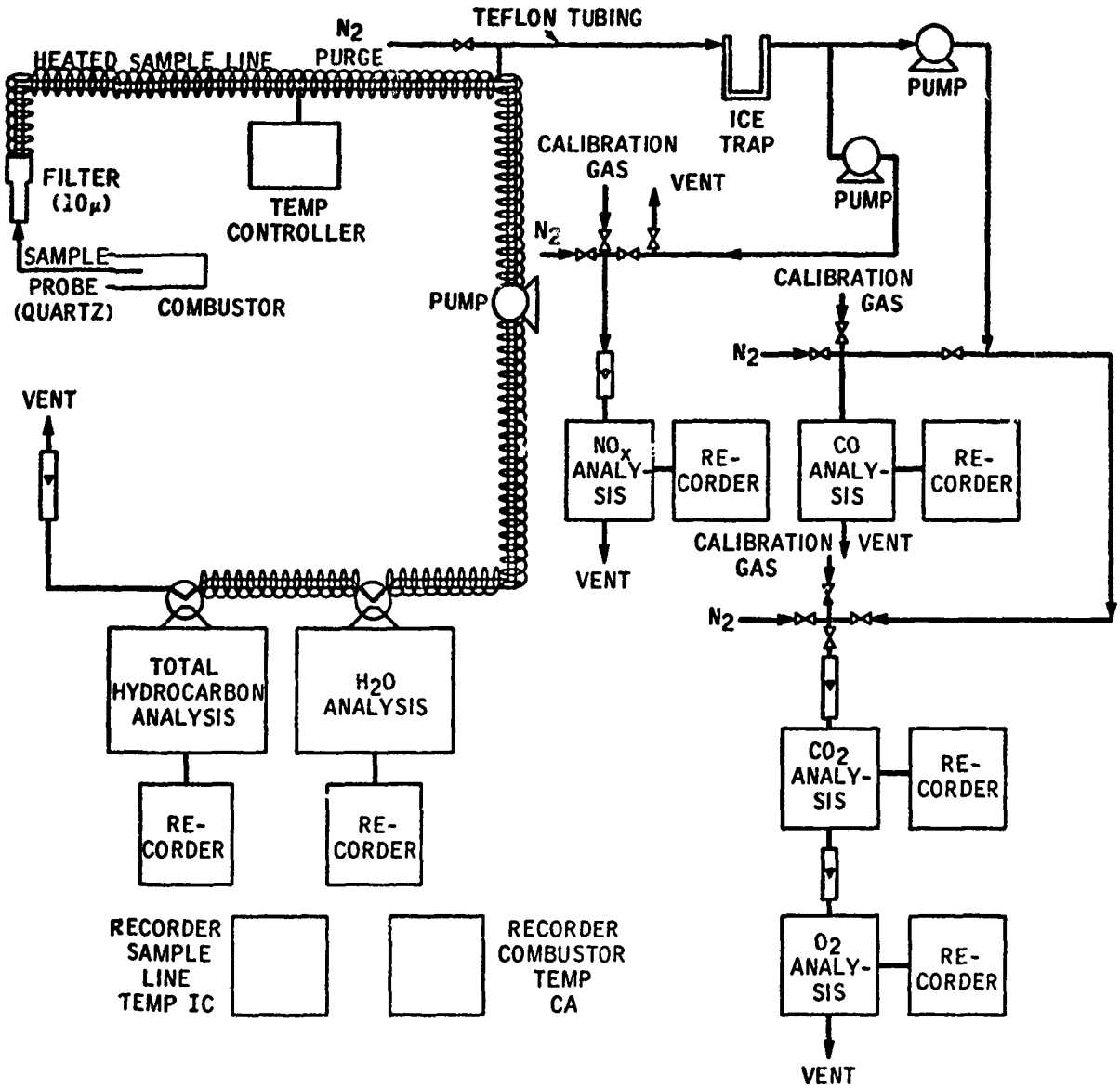

Figure 7

SCHEMATIC OF SAMPLING AND ANALYTICAL SYSTEM

set the temperature of the sampling line. A metal tube was used to hold the Teflon tube and to provide an even temperature distribution which prevented localized burn-out of the Teflon. Because of its inertness, Teflon is an ideal material to prevent any adsorption of gaseous components which would bias the measurements. Sample line temperatures were maintained at 300°F, and were recorded on a strip chart recorder. The heated sample line went directly to the chromatographs. The sample line for the other analyzers tapped off the heated sample line and passed through an ice-trap for water removal. Teflon was used throughout the system.

The CO, CO_2, O_2 and NO_x analytical systems operated continuously and results were recorded permanently on strip chart recorders. The analyses of total hydrocarbons and water were performed chromatographically and depended on instrument response time. The analytical and sampling system completely eliminated the possibility of sample contamination caused by leaks during bottle or bomb storage.

The following analytical techniques were employed:

Total Hydrocarbon. Total hydrocarbons were measured with a flame ionization detector (FID). This method is the most sensitive technique for the detection of hydrocarbons. Detector response is proportional to the number of carbon atoms which can be ionized by the flame per unit time. The technique was developed by removing the GC separation column from an F & M 609 Flame Ionization Temperature Programmed Gas Chromatograph equipped with a strip chart recorder. In order to ascertain whether the oxygen present in the combustion effluent stream affected instrument response (23,24), some calibrations were made with analyzed mixtures of CH_4 in air. No significant difference was detected by using air instead of nitrogen in the premixed calibrating gas. The instrument was calibrated at two hydrocarbon levels using analyzed gas mixture (33 ppm CH_4 in nitrogen and 280 ppm CH_4 in nitrogen).

NO_x. The Nitrogen Oxides were measured using an EnviroMetrics Model N122 continuous analyzer. This is a faradic device with replaceable fuel cell sensors. The gas is absorbed in a surface film and the oxidation/reduction voltage signal produced is proportional to pollutant concentration. Instrument response is linear and up to 90% of full scale within 30 seconds. The analyzer was calibrated using an analyzed gas mixture (100 ppm NO in N_2). The instrument output can be read from the dial and was also recorded on a strip chart recorder. This instrument was purged continuously with nitrogen in order to obtain reproducible results. Readings were, therefore, taken periodically rather than continuously. The EnviroMetric was used to measure total NO_x and NO_2. The NO concentration was determined by difference. In order to ascertain that no interference from other combustion products were observed on the EnviroMetrics analyzer, periodic checks were made with a Thermo Electron and a Bendix chemiluminescent analyzer and a Beckman NDIR analyzer. All NO_x instruments gave results which agreed with the EnviroMetrics to within $\pm$ 5%.

Carbon Dioxide was analyzed continuously using a Beckman Non-Dispersion Infrared Analyzer with a 0-10 vol. % scale readout. The CO_2 readout was recorded on a strip chart recorder. The instrument was calibrated using an analyzed 2 vol. % CO_2 and 100 ppm CO in nitrogen gas blend.

Water was determined on a thermal conductivity P&E 154 gas chromatograph employing a Poropak Q column. A sample of the combustion gas passed continuously through a GC sampling valve, which was used to introduce the sample into the thermal conductivity instrument. The technique was not sufficiently sensitive to distinguish between water emission levels in the air-to-fuel ratio used. The results were generally low by 25%.

Carbon Monoxide was analyzed continuously with a LIRA Infrared Analyzer Model 200 (Mine Safety Appliances). The instrument was calibrated using an analyzed 1000 ppm CO and 10,000 ppm CO mixture in nitrogen.

Oxygen was determined using a Beckman Model 715 Process Oxygen Monitor. This instrument uses a long-life polarographic sensor to measure oxyten. The instrument was calibrated using air.

Tests conducted on the instruments using preanalyzed gas mixtures indicated highly accurate and reproducible measurements of all emissions species of interest.

4. ADDITIVES

The additives were used without further treatment. They were added to measured quantities of fuel in the pyrex fuel tanks and mixed. The modified fuel was pumped through a filter and rotometer into the combustor. The rotometer calibration was checked with each additive and where necessary the fuel rate was corrected for deviations due to the additive. The emulsions that were too viscous to pump conventionally were fed into the combustor using a cylinder with a tightly fitting piston. The emulsion was loaded into the cylinder by hand and sealed. Unmodified fuel was used to drive the piston which in turn forced the emulsion into the combustor.

Over 70 additives were tested in this program. These included 12 metal naphthenates, 6 metal acetylacetonates, 5 metal salts of neoacids, 6 miscellaneous metal compounds, 4 alkali and alkaline earth metal carbonate suspensions, 17 non metal containing additives, and 21 emulsions. Only the additives that showed NO_x reductions of 15% or more were replicated. The variation of metal concentration on NO_x reducing effectiveness was studied for cobalt, iron, copper, and manganese. A detailed description of all the additives tested is included in Tables VI, VII and VIII. The category column refers to the items on pages 15 and 16 in the Introduction.

The metal acetylacetonates (Metal Acac) are not soluble in most common solvents. In order to introduce these compounds into Jet A, a commercial Esso solvent (ECA 9003) was used. This solvent is a mixed C_9 alkyl

TABLE VI

LIST OF FUEL MODIFICATIONS

Metals

Additive	As Received %(w) Metal	Metal Conc. Used Max. %(w)	Metal Conc. Used Min. %(w)	Suppliers Designation	Supplier	Solvent	Symbol	Category
Naphthenate								
Cobalt	6	0.5	0.1	Nap-All Drier	Mooney	Mineral Spirits	CO*NAP	1,3
Cobalt	12		0.1	Neo-Nap Drier	Mooney	High Flash Solvent	CO*NAP	1,3
Calcium	4		0.1	Nap-All Drier	Mooney	Mineral Spirits	CA*NAP	1,3
Copper	8	0.5	0.1	Nap-All Drier	Mooney	Mineral Spirits	CU*NAP	1,3
Iron	6	0.2	0.1	Nap-All Drier	Mooney	Mineral Spirits	FE*NAP	1,3
Manganese	6	0.2	0.1	Nap-All Drier	Mooney	Mineral Spirits	MN*NAP	1,3
Manganese	9	0.2		Neo-Nap Drier	Mooney	High Flash Solvent	MN*NAP	1,3
Zinc	10	0.2		Nap-All Drier	Mooney	Mineral Spirits	ZN*NAP	1,3
Chromium	4.0		0.1	--	ROC/RIC	None	CR*NAP	1,3
Vanadium	1.08		0.1	--	ROC/RIC	None	V*NAP	1,3
Nickel	5.6		0.1	--	ROC/RIC	None	NI*NAP	1,3
Cerium	12.7		0.1	--	ROC/RIC	None	CE*NAP	1,3
Lead	24	0.5		Nap-All Drier	Mooney	Mineral Spirits	PB*NAP	1,3
Acetyl Acetonates								
Ferric	15.8		0.1	--	ROC/RIC	Alkyl Phenol	FE*ACAC	1,3
Aluminum	8.3		0.1	--	ROC/RIC	Alkyl Phenol	AL*ACAC	1,3
Cupric	25.2		0.1	--	ROC/RIC	Alkyl Phenol	CO*ACAC	1,3
Cobaltic	16.7		0.1	--	ROC/RIC	Alkyl Phenol	CO*ACAC	1,3
Cobaltous	23.9		0.15	--	ROC/RIC	Alkyl Phenol	CO*ACAC	1,3
Nickel	22.9		0.1	--	ROC/RIC	Alkyl Phenol	NI*ACAC	1,3
0.7 Ni/0.3 Cu ("Monel")	--		0.1	--	ROC/RIC	Alkyl Phenol	MONEL*ACAC	1,3,7
Salt of Neo Acids								
Cobalt	12	0.2		Ten-Cem Drier	Mooney	Neodecanoic Acid	CO*NEO	1,3
Zirconium	18	0.2	0.1	Ten-Cem Drier	Mooney	Neodecanoic Acid	ZR*NEO	1,3
Zirconium	12	0.2		Cem-All Drier	Mooney	C_8 to C_{14} Neo Acid	ZR*NEO	1,3
Vanadium	6	0.2		Ten-Cem Drier	Mooney	Neodecanoic Acid	V*NEO	1,3
Lithium	2		0.1	Ten-Cem Drier	Mooney	Neodecanoic Acid	LI*NEO	1,3

TABLE VI (Cont'd.)

Additive	As Received %(w) Metal	Metal Conc. Used Max. %(w)	Metal Conc. Used Min. %(w)	Suppliers Designation	Supplier	Solvent	Symbol	Category
Miscellaneous Metals								
Sodium Methoxyethoxy-aluminum Hydride	70	0.13		SDMA	ROC/RIC	Benzene	SDMA	1,2,3
Tetraethyl Lead	64		0.18	--	Esso	None	PB*TEL	1,3
Methyl Cyclopenta-dienyl Manganese	24.7	0.5	0.1	CI-2	Ethyl	None	MN*CI2	1,3
Iron	30.0	0.5	0.1	Ferrocene	ROC/RIC	None	FE*FERROCENE	1,3
Antimony Triphenyl	34.6		0.1	--	ROC/RIC	None	SB*3C6H5	1,3
Copper-Phosphine Complex	20		0.1	--	Esso	None	CU*PHOS	1,3
Suspensions								
Sodium Carbonate	17		0.1	ECA-5202	Esso	Diluent Oil	NA*S	1,2,3
Calcium Carbonate	12		0.1	ECA-4651	Esso	Diluent Oil	CA*S	1,2,3
Lithium Carbonate	1		0.1	Experimental	Esso	Diluent Oil	LI*S	1,2,3
Barium Carbonate	17		0.1	Paradyne 12	Esso	Diluent Oil	BA*S	1,2,3

TABLE VII

LIST OF FUEL MODIFICATIONS

Emulsions

Additive	Internal to External Phase Vol. Ratio	External Phase %(w) Water	Emuls.	Additive	Supplier Designation	Supplier	Symbol	Category
Water	97:3	74.7	25.3	--	EFA-104A	Petrolite	3.8 H2O*E	3
Water + Methanol	97:3	59.7	25.3	15.0	EFA-104B	Petrolite	3.8 H2O+CH3OH*E	3,4
Water + Ammonium Formate	97:3	74.7	25.3	0.1	EFA-104C	Petrolite	3.8 H2O+NH4CHO2*E	3,6
Water + Ammonium Nitrate	97:3	74.7	25.3	0.1	EFA-104D	Petrolite	3.8 H2O+NH4NO3*E	3,6
Water + Hydrazine Acetate	97:3	74.7	25.3	0.1	EFA-104E	Petrolite	3.8 H2O+N2H4·2C2H4O2*E	3,6
Water + Amine	97:3	74.7	25.3	0.1	EFA-104F	Petrolite	3.8 H2O+B4367*E	3,6
Water + Ammonium Molybdate	97:3	74.7	25.3	0.1	EFA-104G	Petrolite	3.8 (NH4)2MOO4*E	3,6
Water 3.3%(w)	97:3	76.7	23.3	--			3.3 H2O*E	3
Water 5.0%(w)	95:5	83.6	16.4	--			5.0 H2O*E	3
Water 10.0%(w)	91:9	90.9	9.1	--			10.0 H2O*E	3
Water 20.0%(w)	81:19	95.3	4.7	--			20.0 H2O*E	3
Water 33.3%(w)	71:29	97.1	2.9	--			33.0 H2O*E	3
Methanol	99:1	--	75.1	24.9			0.33 CH3OH*E	3,4
Water + Ammonium Hydroxide	99:1	6.3	91.0	2.7			0.07 H2O+NH3*E	3,6
Water + Hydrazine	97.4	68.6	20.9	10.5			3.5 H2O+N2H4*E	3,6
100:10:1 Water:Methanol: Ammonia	96:4	71.4	21.2	7.3			3.3 H2O+CH3OH+NH3*E	3,6
Water + Lithium Hydroxide	94:6	75.6	23.8	0.5			5.8 H2O+LIOH*E	3,2,1
Water + Sodium Hydroxide	96:4	60.8	38.3	1.0			3.0 H2O+NaOH*E	3,2,1
Water + Potassium Hydroxide	94:6	75.4	23.8	0.8			5.8 H2O+KOH*E	3,2,1
Water + Rubidium Hydroxide	96:4	59.8	37.7	2.5			3.0 H2O+RBOH*E	3,2,1
Water + Cesium Hydroxide	94:6	74.4	23.4	2.2			5.8 H2O+CSOH*E	3,2,1

TABLE VIII

LIST OF FUEL MODIFICATIONS

Homogeneous Additives

Additive	Concentration % W	Concentration % V	Supplier Designation	Supplier	Symbol	Category
Ethylene Ether Dimethyl Glycol	3.5	2.5		Fisher Scientific	3.5 EGDE*H	4
Benzene	2.7	2.5		Allied Chemical	2.7 C6H6*H	4,3
Carbon Tetrachloride	5.0	2.5		Allied Chemical	5.0 CCL4*H	2
Ethanol	2.5	2.5		Commercial Solvents	2.5 C2H5OH*H	4
Propyl Nitrate		2.5		Eastman Organic	3.7 C3H7NO3*H	5
Aniline	3.2	2.5		Allied Chemical	3.2 C6H5NH2*H	4
Polyisobutylene	2.7	2.5	Vistonex J	Esso	3.1 POLY*H	5
Dicyclopentadiene	2.9	2.5		Matheson, Coleman Bell	2.9 DCPD*H	3
Hexafluoropropenol	5.6	2.5		Matheson, Coleman Bell	5.6 C3F6HOH*H	2
C_{13} Branched Amine	2.7	0.5		Esso	0.5 C13NH2*H	6
Solvent for Cem-All Metals	9.1		Cem-All Solvent	Mooney	9.1 CEM All*H	--
Solvent for Ten-Cem Metals	9.1		Ten-Cem Solvent	Mooney	9.1 TEN CEM*H	--
Solvent for Neo-Nap Metals	9.1		High Flash Solvent	Mooney	9.1 HFL*H	--
Solvent for Nap-All Metals	9.1		Mineral Spirits	Mooney	9.1 MS*H	--
N,N,N,N, Tetramethylamine	.62	0.55		Esso	0.55 TMA*H	6
N-Butyl Mercaptan	2.6	2.5		Matheson, Coleman Bell	2.6 C4H9SH*H	2

phenol containing 65% monoalkyl phenol and 35% dialkyl phenol. The metal was generally dissolved to approximately 2% in the alkyl phenol and then diluted to the desired concentration in Jet A. As much as 5% of the fuel was alkyl phenol when the metal acetylacetonates were run.

The Petrolite emulsions contained a proprietary nonionic emulsifier blend called Tech Mul-2. The emulsifiers are oxyalkylates of linear and branched alcohols and they contain only carbon, hydrogen and oxygen in their makeup. The compound b-4367 is a proprietary antioxidant described as an oxyalkylated amine containing approximately 25% nitrogen in its composition the remainder being carbon, hydrogen and oxygen.

The Esso prepared emulsions contained a mixture of Tween 20 and Span 80. These emulsifiers are manufactured by Atlas Chemical Industries. They contain only carbon, hydrogen and oxygen.

SECTION IV

RESULTS

Experiments were run over the equivalence ratio range of 0.27 to 0.34. Equivalence ratio, ϕ, is the ratio of stoichiometric air to fuel ratio to operating air to fuel ratio. This range of equivalence ratios corresponds to aircraft engine operation at full power. Experimental results were obtained under the operating conditions listed in Table V. The equivalence ratio values were calculated on a stoichiometric air to fuel ratio of 14.6 (by weight) which corresponds to a fuel with a hydrogen to carbon ratio of 1.89. The hydrogen to carbon ratio for Jet A was determined experimentally using a very accurate combustion technique and measuring the CO_2 and H_2O produced. The ratio is 1.89 ± 0.08 at the 95% confidence level. Measurements of impurities in the fuel indicated that the percent oxygen is 0.38, the percent sulfur is 0.05, and the percent nitrogen is 0.00. The contribution of fuel nitrogen, assuming that the fuel contained 0.005% nitrogen and it was all converted to NO_x, would be 0.16 lb of NO_x (as NO_2) per 1000 lb of fuel.

The material balance calculations and the treatment of the data are explained in Appendix V. The experimental mole fraction values for CO_2, CO, O_2 and NO_x were multiplied by a factor $(1.0 - 0.132\phi)$ in order to compensate for the water removed in the ice bath.

1. EMISSIONS WITH UNMODIFIED FUEL

In order to measure the effectiveness of the fuel modifications tested, 93 runs were interspersed with unmodified Jet A fuel. The results of these runs were subjected to a statistical analysis in order to obtain the least squares relationships between the various components of the flue gas and equivalence ratios.

The least squares relationships that were obtained with unmodified Jet A fuel are listed in Table IX for Can I and in Table X for Can II. The data in these tables are based on a linear regressions of the 93 separate runs that were made over the duration of the experimental phase of this program. The experimental data are given in Appendix IV.

All these equations apply only within the limited range of the experimental work. The tolerance limits on the slope of the least squares lines were calculated by multiplying the appropriate Student's t value by the standard error of the estimate. The average carbon balance for unmodified Jet A combustion was 96.3% and the average oxygen balance was 98.8%.

TABLE IX

LEAST SQUARES RELATIONSHIPS FOR CAN I

Linear Equation	Constraint	% Variation at 95% Confidence Level
% CO_2 = $(12.2 \pm 0.3)\phi$	Constant = 0	2.6
% O_2 = (20.1 ± 0.9) $(1-\phi)$	Variable = $(1-\phi)$ Constant = 0	4.7
ppm CO = $-(11.9 \pm 1.8)$ 1000ϕ + 6400	none	15.3
ppm HC = (18.1 ± 1.5) 100ϕ - 508	none	8.3
ppm NO_x = (18.6 ± 0.8) 10ϕ + 29.6	none	4.3
ppm NO_2 = $(55.8 \pm 3.8)\phi$ - 2.24	none	6.8
Te, °F = (24.6 ± 0.6) 100ϕ + 768	none	2.5
Tp, °F = (23.7 ± 0.6) 100ϕ + 808	none	2.6

TABLE X

LEAST SQUARES RELATIONSHIPS FOR CAN II

Linear Equation	Constraint	% Variation at 95% Confidence Level
$\% CO_2 = (12.2 \pm 0.4)\phi$	Constant = 0	3.4
$\% O_2 = (20.8 \pm 0.7)(1-\phi)$	Variable = $1-\phi$ Constant = 0	3.4
ppm CO = $-(47.1 \pm 1.6)\ 1000\phi + 18100$	none	3.5
ppm HC = $-(22.2 \pm 1.8)\ 10\phi + 86.5$	none	8.0
ppm NO_x = $(34.4 \pm 1.1)\ 10\phi + 23.0$	none	3.1
ppm NO_2 = $(17.8 \pm 0.8)\ 10\phi + 34.1$	none	4.4
Te, °F = $(33.5 \pm 7.8)\ 100\phi + 516$	none	2.3
Tp, °F = $(30.9 \pm 7.2)\ 100\phi + 597$	none	2.3

In order to provide a convenient source for comparison of the emission levels determined here with those from actual aircraft engines the mole fraction values were converted to emission index units and are reported in Table XI.

TABLE XI

AVERAGE VALUES OF EMISSION INDEX AND TEMPERATURES FOR UNMODIFIED JET A COMBUSTION

Parameter	Emission Index lb/1000 lb	Standard Deviation
Carbon Dioxide	2772	139
Oxygen	7598	610
Carbon Monoxide	147	53.4
Unburned Hydrocarbons as Methane	0.843	1.38
Oxides of Nitrogen (as Nitrogen Dioxide)	6.55	0.404
Nitrogen Dioxide	1.55	0.352
Exit Temperature, °F	1555	62.3
Probe Temperature, °F	1554	56.1

The method for converting mole fraction values to emission index is described in Appendix V and is based on equation (8).

$$EI_i = X_i \left[\frac{n\phi + 4.76\ (4 + n)}{4.76\ (4 + n)} \right] \frac{14.7}{\phi} \times \frac{(MW)_i}{29} \times 10^3 \qquad (8)$$

where:

X_i = mole fraction of i.

EI_i = Emission index in lb of i/1000 lb fuel.

n = Atomic hydrogen to carbon ratio of the fuel = 1.89 for Jet A.

ϕ = Equivalence ratio

$(MW)_i$ = Molecular weight of i.

The average emission index for carbon monoxide was more than an order of magnitude higher than those reported from actual engine emissions measurements (13,14,15). This high level of carbon monoxide is attributed to less efficient mixing in the Esso combustor as measured by the low pressure drop through the combustor. In general, aircraft combustors have a 5% pressure drop (Δ P/P) while the pressure drop in the laboratory unit was about 1%.

A reference set of emissions was calculated for each fuel modification run using the least squares lines. These reference emission were used to calculate the change of emission levels due to the modification. The reference set of emissions is tabulated in Appendix II. Figure 8 is a plot of NO_x mole fraction in the effluent as a function of equivalence ratio. The least squares line is that given in Table X and the calculated line is based on equation (6) assuming that combustion occurs at an equivalence ratio of 1.0 and fuel flow rate sets the residence time in the primary zone. The primary zone residence time at an overall equivalence ratio of 0.27 is 1.5×10^{3} seconds which was calculated assuming an L/D of 0.5. Calculational details are given in Appendix VI.

In addition to the least squares regression reported in Tables IX and X, the degree of linear relationship between the measured parameters and NO_x was determined. The statistical measure of the degree of relationship between two variables is called the correlation coefficient and is defined as the square root of the ratio of the explained variation to the total variation (25). A correlation coefficient of 0.8 means that 64% of the variation is accounted for by the least squares line. The other 36% must be accounted for by other factors. The simple correlation coefficients listed in Table XII were obtained from runs 1 to 42 using Can I, and from runs 43 to 93 using Can II. The minimum value of the simple correlation coefficient at the 95% confidence level for the number of experiments that were run is also included in Table XII.

Other parameters such as inlet air moisture and combustor pressure did not correlate significantly with NO_x.

2. EMISSIONS FROM MODIFIED FUEL

Approximately 70 fuel modifications were tested using Jet A as the base fuel. These fell into the 7 categories mentioned in the Introduction. Only category 1 proved to be effective in reducing oxides of nitrogen emissions. The results with transition metals are presented in Figure 9. The mechanism for NO_x reduction with transition metals was not determined but seems to parallel results that have been observed in heterogeneous catalytic systems (26). Figure 9 shows that the logarithmic activity of some transition metal oxides for NO decomposition follows a similar trend to that observed with the transition metal additives that were tested in this program. The contribution due to the organic ligands was neglected as a first

TABLE XII

CORRELATION OF NO_x WITH OTHER EMISSIONS AND TEMPERATURES

Parameter	Simple Correlation Coefficient (r)			
	Can II		Can I	
	Calculated	Min. Required	Calculated	Min. Required
Equivalence ratio, ϕ	0.678	0.276	0.650	0.304
CO_2, %	0.865	0.281	0.703	0.304
O_2, %	0.678	0.273	0.650	0.320
CO, ppm	0.685	0.276	0.553	0.304
NO_2, ppm	0.643	0.276	0.647	0.482
Te, °F	0.901	0.301	0.736	0.304
Tp, °F	0.838	0.295	0.678	0.304

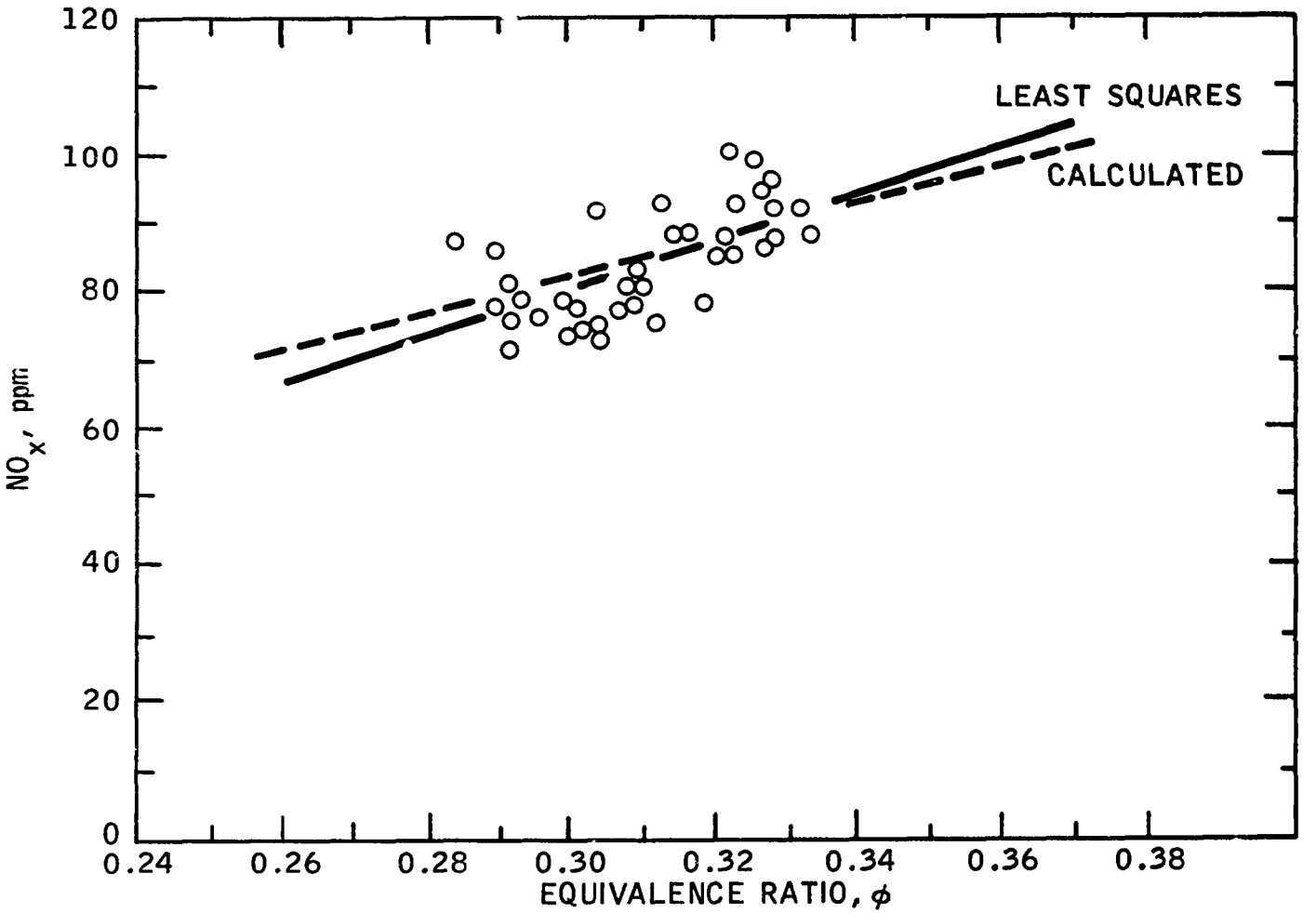

Figure 8

COMPARISON OF CALCULATED AND LEAST SQUARES RELATIONSHIP OF NO_x FROM UNMODIFIED JET A AS A FUNCTION OF EQUIVALENCE RATIO

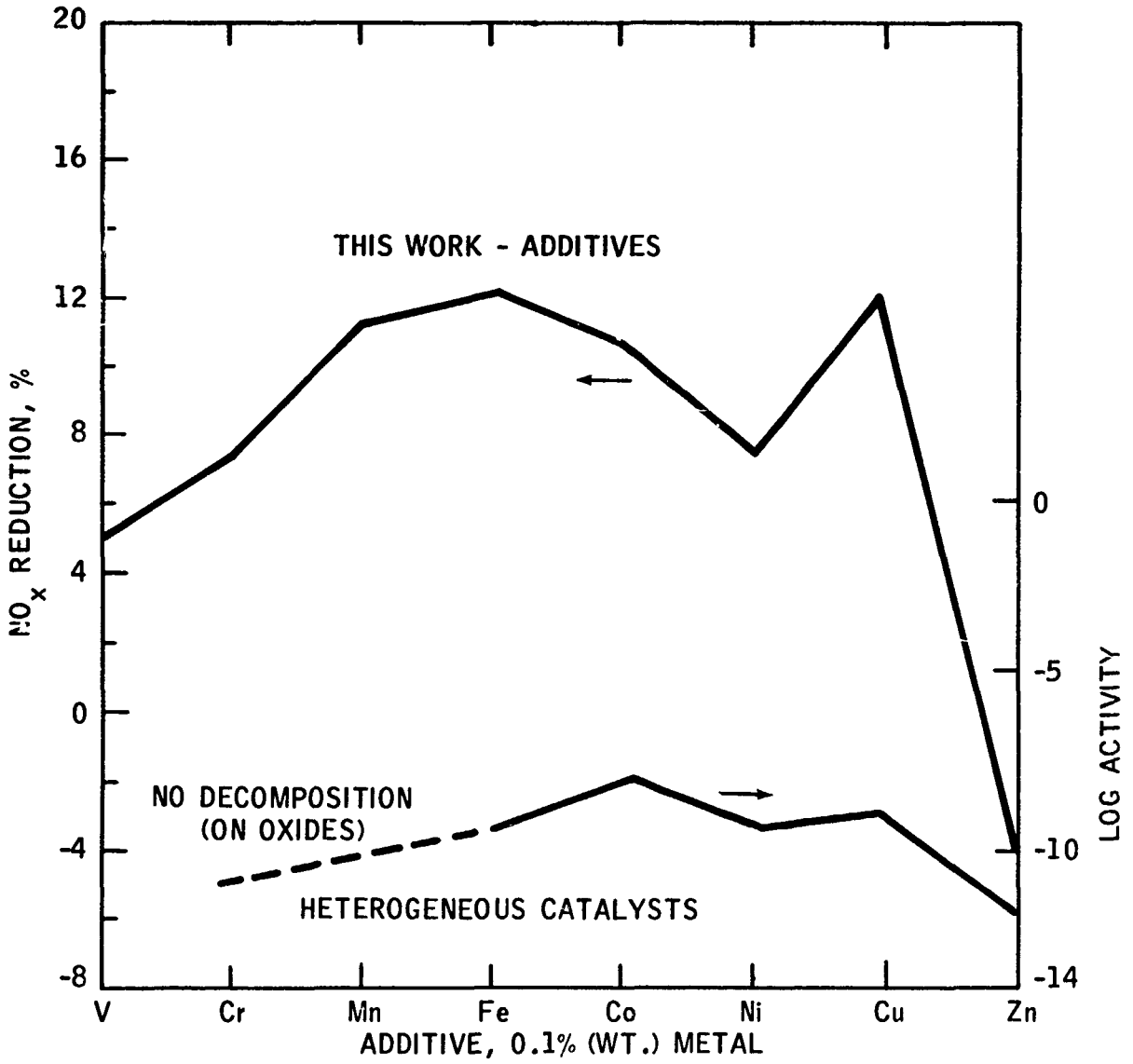

Figure 9

NO_x REDUCING ABILITY OF TRANSITION METAL ADDITIVES AND HETEROGENEOUS CATALYSTS

approximation in plotting these results. The four most effective metals were studied as a function of treat rate. The data for manganese and iron are shown in Figure 10 and the data for cobalt and copper are shown in Figure 11. All four metals became less effective per incremental treat rate increase. The only other effective metal was zirconium which reduced NO_x by 11% at a 0.1% (w) treat rate and 22% at a 0.2% (w) treat rate. Other organometallic compounds containing calcium, cerium, lead aluminum, lithium, and antimony did not reduce NO_x significantly at the 0.1% (w) metal treat rate.

Four suspensions of metal carbonates were run at 0.1% (w) metal treat rate. Sodium carbonate reduced NO_x by about 16% and lithium carbonate by about 10%. The other carbonates, barium and calcium, were not effective.

Out of the 16 homogeneous (soluble liquid additives) fuel modifications only n-butyl mercaptan was effective. The mercaptan reduced NO_x by almost 11%. The nitrogen containing compounds increased NO_x in proportion to their nitrogen content. Approximately 25% of the nitrogen was converted to NO_x. As the treat level of nitrogen containing additives was reduced, the conversion of nitrogen to NO_x decreased at a greater rate than the reduction in treat level. This effect was not fully explored. The homogeneous additives tested include ethylene ether dimethyl glycol, benzene, carbon tetrachloride, ethanol, propyl nitrate, aniline, polyisobutylene, dicyclopentadidne, hexafluoropropanol, a C_{13} branched amine, N,N,N,N-tetramethylamine, and N-butyl mercaptan.

A number of water emulsions were run in order to determine the effect of water in reducing NO_x. Water emulsions also provide a convenient vehicle for introducing inorganics into the fuel. Emulsions were run with up to 33% (w) water. No reduction in NO_x was observed as a function of equivalence ratio. The only effect was an increase in the NO_2 to NO_x ratio as shown in Figure 12. A series of water emulsions containing equal molar concentrations of the alkali metal hydroxides gave the results plotted in Figure 13. Sodium proved to be the most effective additive in this series. The only other water emulsion that showed some promise in reducing NO_x was one that contained 37 ppm (w) hydrazine acetate. The runs with this emulsion were erratic but some replicates gave as much as 16% NO_x reduction. The emulsions which were ineffective were methanol, ammonium formate, ammonium nitrate, ammonium molybdate, ammonium hydroxide, and hydrazine.

Some runs were made with a combination of additives from two categories in an attempt to see whether synergistic effects are possible. Antimony triphenyl and carbon tetrachloride reduced NO_x by 12% which was in excess of the reduction obtained with these additives separately.

A simple way of ranking the effectiveness of the fuel modifications was developed. The effectiveness of the additives was measured in terms of the number of molecules of NO_x reduced per molecule of additive. Some of the more effective modifications are listed in Table XIII.

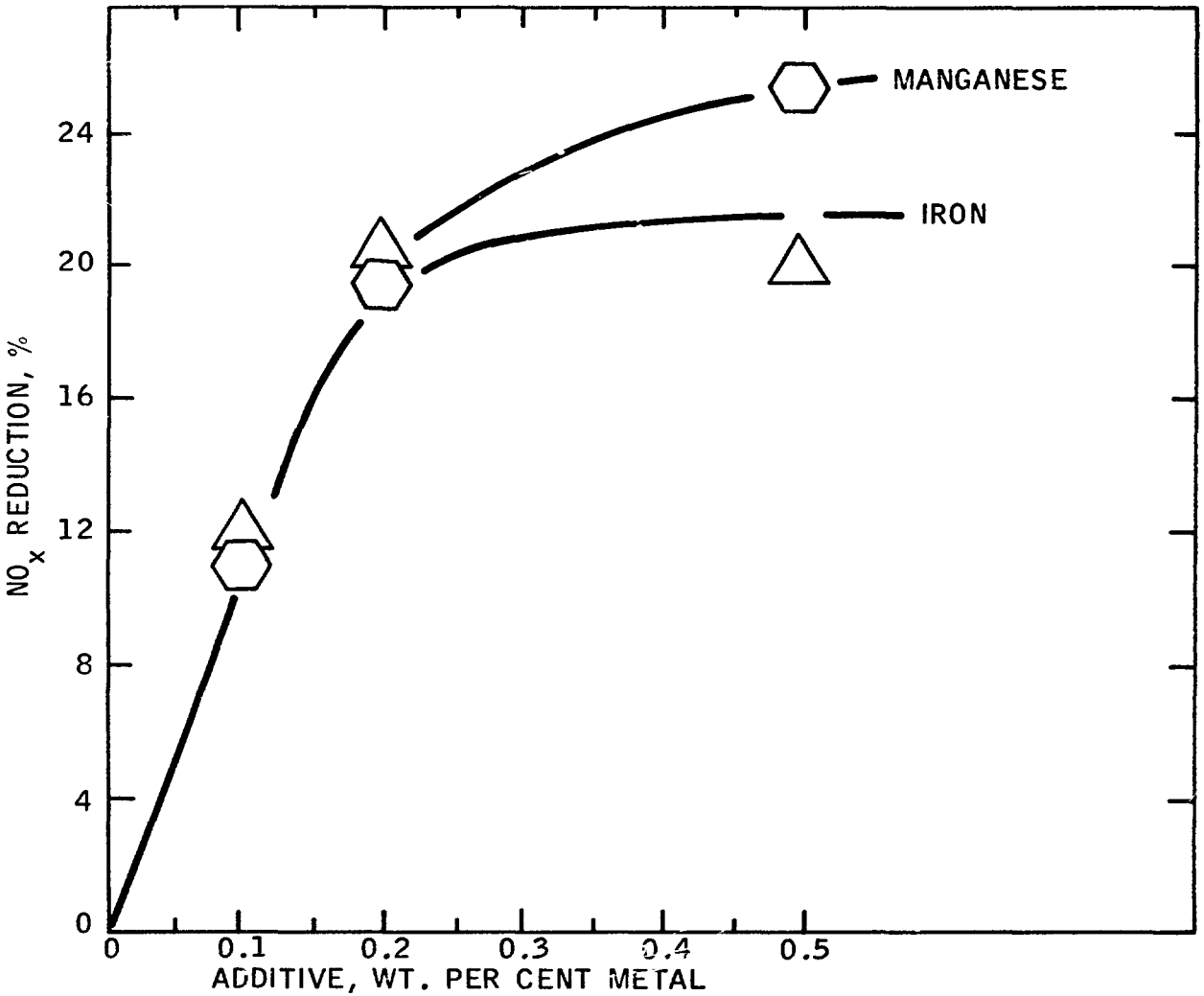

Figure 10

EFFECT OF CONCENTRATION ON NO_x REDUCING ABILITY OF IRON AND MANGANESE ADDITIVES

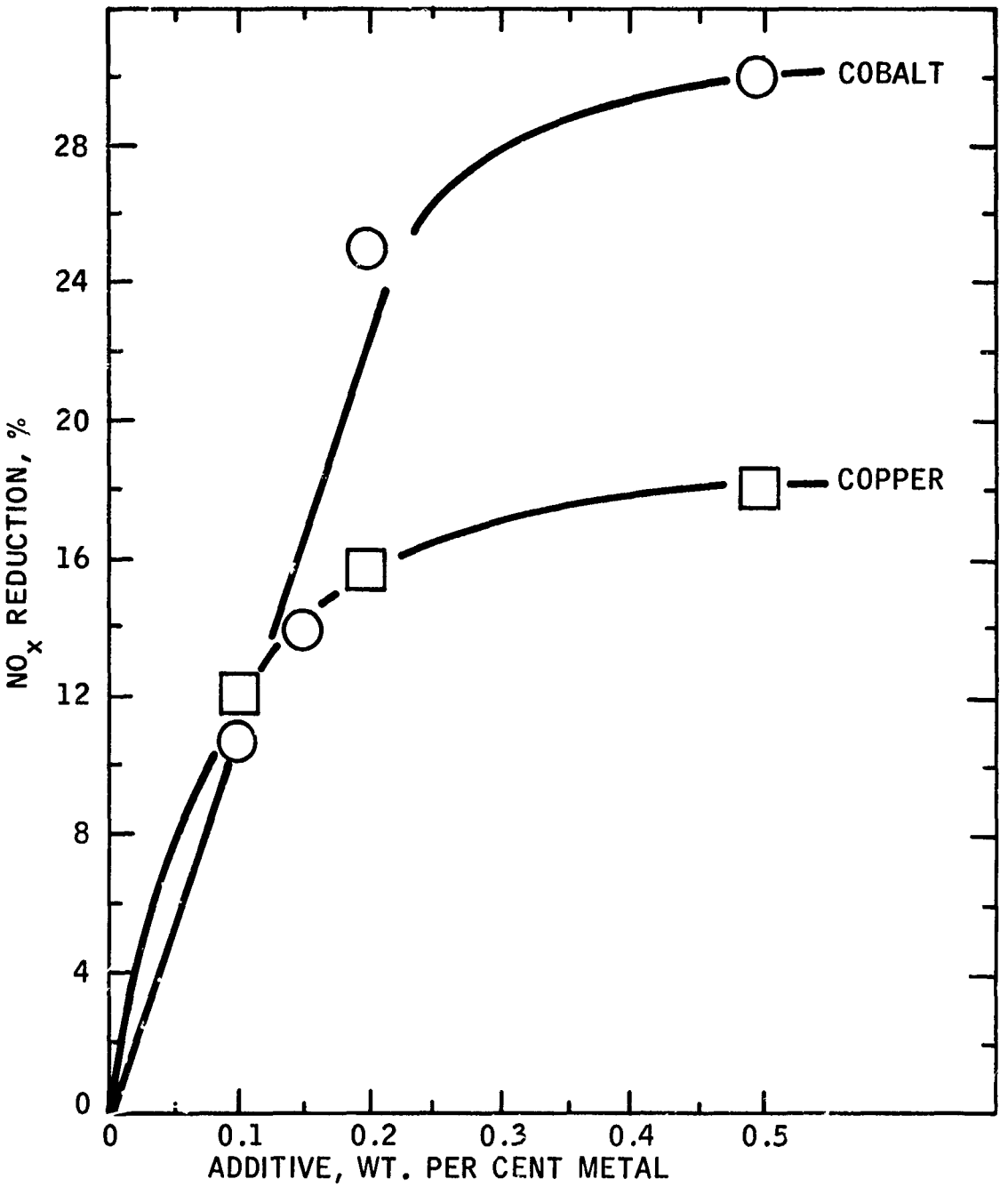

Figure 11

EFFECT OF CONCENTRATION ON NO_x REDUCING ABILITY OF COPPER AND COBALT ADDITIVES

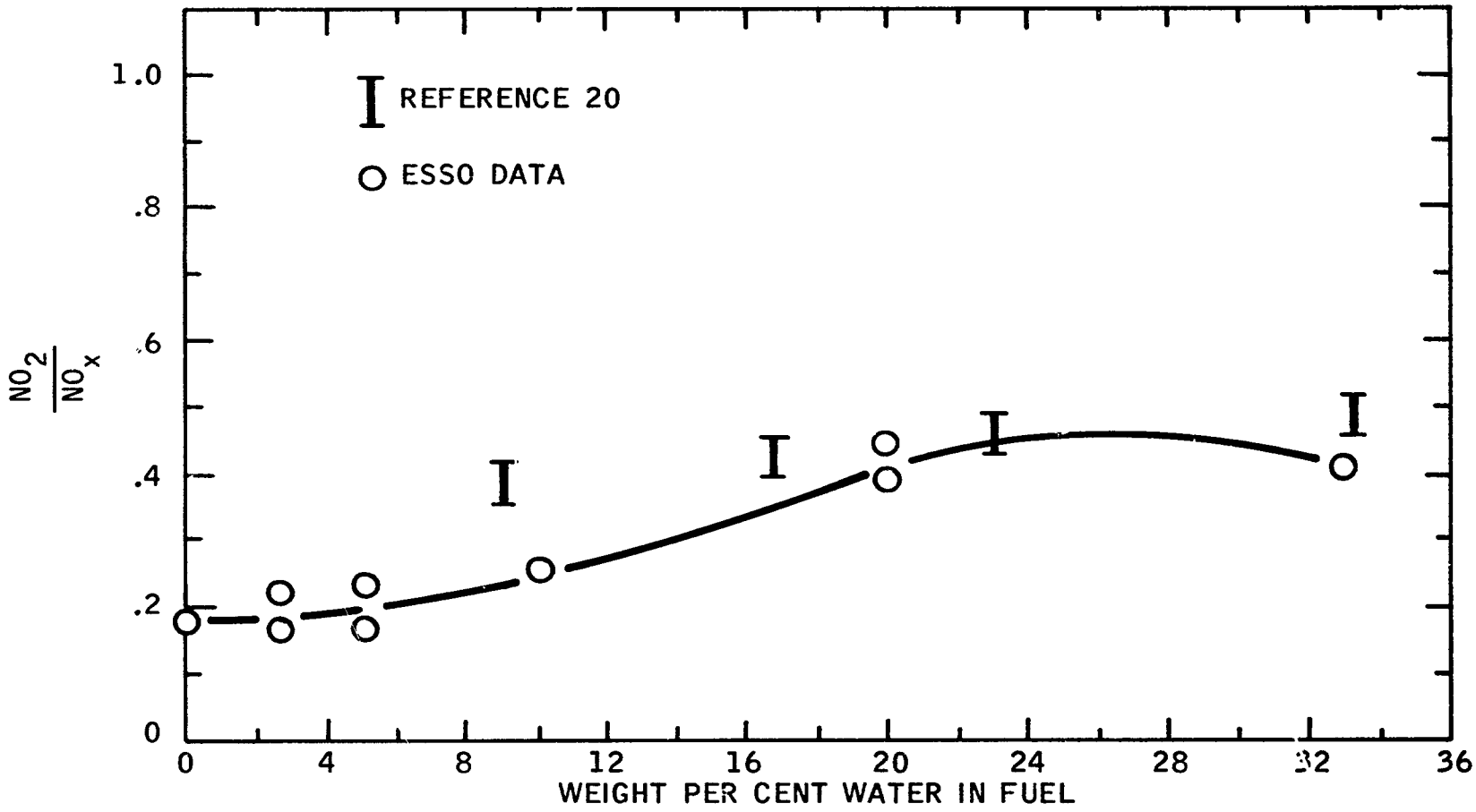

Figure 12

EFFECT OF WATER ON THE NO_2 TO NO_x RATIO

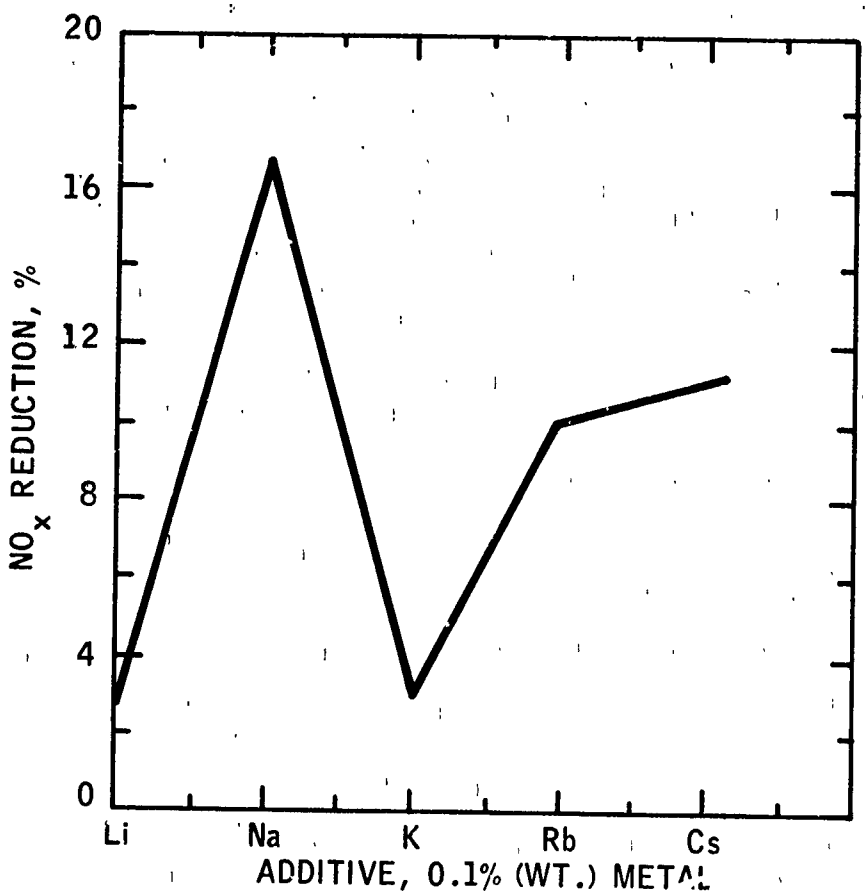

Figure 13

NO_x REDUCING ABILITY OF ALKALI METAL HYDROXIDE WATER EMULSIONS

TABLE XIII

NO_x REDUCING EFFECTIVENESS OF VARIOUS ADDITIVES

Δ NO_x MOLECULE / MOLECULE ADDITIVE	ADDITIVE IN PER CENT (W)		% REDUCTION NO_x
90	0.0037	HYDRAZINE ACETATE IN WATER EMULSION	15
1.7	0.1	MANGANESE NAPHTHENATE	20
1.5	0.1	COBALT ACETYLACETONATE	17
1.4	0.1	COPPER NAPHTHENATE	15
1.4	0.2	IRON NAPHTHENATE	35
1.0	0.1	IRON NAPHTHENATE	12
.9	0.1	SODIUM CARBONATE SUSPENSION	26
.9	0.2	COBALT NAPHTHENATE	25
.8	0.2	COPPER NAPHTHENATE	16
.5	0.5	COBALT NAPHTHENATE	30

SECTION V

DISCUSSION

The fuel modification experimental program was designed to be a broad based search for NO_x reducing additives. Practical limitations to the use of these additives in actual aircraft engines were relegated to secondary importance in order not to obscure potentially interesting leads. The potentially useful approaches to the problem were classified into 7 general categories which were described in the Introduction. These categories were selected so as to systematize the search for additives and/or modifications based on theory and prior art and to avoid a pure trial and error approach. As indicated in the results section, the organometallic compounds of some of the transition metals proved most effective in reducing NO_x. The mechanism for NO_x reduction with transition metals was not determined but seems to parallel results that have been observed in heterogeneous catalytic systems (26).

The catalysts that have been used to affect either the decomposition or reduction of nitrogen oxide have been heterogeneous catalysts. A bed of solid catalyst or a screen of catalyst wire was contacted with the nitrogen oxide containing gases. The metal and/or metal oxide catalysts which are active for NO conversion are insoluble in jet fuel. Organometallic compounds were added to the fuel as soluble compounds or when not soluble an organic carrier was used to maintain these compounds in solution. Upon entry into the combustion zone, these compounds are expected to form a highly dispersed heterogeneous catalyst. Indeed, in some experiments with iron compounds a red brown powder was found on the combustor can which was assumed to be iron oxide. Similarly, other metals seemed to leave traces of their oxides on the combustor can.

The introduction of metal containing compounds into the combustor of a gas turbine engine can cause serious operational problems. Deposits can be formed which could produce "hot spots" resulting in erosion and corrosion of the liner and turbine vanes. In addition, organometallic compounds are known to accelerate the formation of sediment in aircraft fuels. The sediment can plug narrow passages and foul heat transfer surfaces rendering an aircraft inoperable (27). These detrimental factors were not considered in choosing fuel modifications in order not to miss any leads to potentially promising approaches.

The mechanism and kinetics of NO formation in flames makes its production extremely sensitive to the time-temperature-history of the combustion process, and the oxygen concentration in the flame zone. Consequently, fuel additives or changes in composition capable of altering these factors could have a pronounced effect on the NO emission from jet engines.

The rate at which NO is formed from molecular nitrogen at high temperature depends upon the availability of atomic oxygen for reaction (2). Other factors being equal, any reduction in the concentration of atomic oxygen decreases the rate of NO formation and hence its emissions.

A reduction in atomic oxygen availability can be produced by using compounds capable of reacting with oxygen atoms or catalyzing their recombination. Compounds possessing these properties are known and have been studied and used for their flame inhibiting properties which also depend on the ability to scavenge or recombine oxygen. Some of the more effective compounds known for their flame inhibiting characteristics include the halogen gases (with the exception of florine), certain organo-halogen compounds such as CF_3Br and CF_3COCF_3, alkali metal oxides and carbonates, and certain organometallic compounds.

The metal oxides and carbonates act through the formation of metal peroxides by a mechanism involving atomic oxygen. This is in line with the fact that both the ease of formation and the stabilities of peroxides of the alkali metals increase with molecular weight as do the extinguishing efficiencies of the oxides and carbonates (28). In the series of alkali metal hydroxide solutions that were added to jet fuel as emulsions, sodium was found to be most effective. With this exception, the trend with molecular weight was followed with the other alkali metal hydroxides.

Out of the four carbonate suspensions that were tested, only the alkali metal carbonates were effective. Sodium carbonate reduced NO_x by 16% and lithium carbonate by 10%.

The effectiveness of the organometallics may be due to their ability to scavenge oxygen atoms rather than catalyze NO decomposition. No data is available to rule in favor of one mechanism over the other but some metals such as aluminum, which would be expected to scavenge oxygen atoms, did not reduce NO_x. On the other hand, this result is consistent with the inability of alumina to catalytically reduce or decompose NO_x (29).

Besides the halogen and metal containing compounds, soot (i.e., smoke) could also prove effective for promoting the recombination of oxygen atoms. Addition to the fuel of such soot precursors as benzene and dicyclopentadiene did not, however, reduce NO_x emissions.

Using fuel additives to produce lower combustion temperatures provides another technique for reducing NO emissions. Since the rate of NO formation from molecular nitrogen and oxygen is so extremely temperature dependent (see Appendix VI), small changes in peak combustion temperatures significantly affect NO formation. In gas turbine engines, peak temperatures are normally reached in the vicinity of the primary combustion zone where close to stoichiometric air/fuel conditions are achieved. Consequently, it is in this part of the engine where reductions in temperature would have their greatest impact in reducing NO formation.

Peak combustion temperatures in jet engines can be reduced by increasing the radiative heat transfer characteristics of the primary zone. Any particulate matter in the flame, including soot, would increase the amount of heat radiation from the flame. Increasing the CO_2 content of the gas would also increase its radiative character. This category (category 3 in list) proved ineffective since all organometallic additives increased the solids loading in the flame yet some metallo-organics were effective NO_x reducers while others were not. Thus, one cannot attribute any significant reduction in NO_x to a radiative heat transfer mechanism.

A second potential method of reducing peak combustion temperatures in the jet engine would be to add compounds to the fuel capable of undergoing endothermic physical or chemical conversions within the primary zone of the jet engine. This could involve adding compounds to the fuel that are likely to undergo such reactions. Of course, the heat absorbed by the endothermic reaction in the fuel rich primary zone would be released in the cooler secondary zone as long as combustion was completed there. Thus, combustion efficiency need not suffer with this approach.

Water is generally considered the prime candidate additive capable of undergoing endothermic physical changes. Since the vaporization of water removes approximately 1000 Btu/lb compared to a fuel heating value of about 18,400 Btu/lb, water addition to the fuel would produce only small changes in combustion temperatures unless it were used in prohibitively large amounts. However, even small changes in jet engine peak temperatures may be sufficient to cause substantial changes in NO_x emissions. This fuel modification proved ineffective in this program even with water levels of 33% (w) of the fuel. On the other hand, an increase in the NO_2 to NO_x ratio is indicative of a reduction in operating temperature. As can be seen in Figure 14 the NO_2:NO_x ratio, calculated from equilibrium data (5), increases as temperature decreases under fuel lean operation. A recent paper evaluating the effect of water in gas turbines was presented by Lipfert (30). He shows that the effect of water is a function of the water to air ratio (by mass) and that relatively small effects are produced by water to air ratios of less than 0.01. Since 33% (w) water in fuel correponds to less than 0.007 lb water per lb of air, it is not surprising that no effect due to water was observed. Also, Boccio, Weilerstein and Edelman (31) recently showed that the effectiveness of water emulsions in reducing NO_x is a function of droplet size and residence time in the primary zone. Using the correlations presented by Boccio et al for conditions that are assumed representative of the Esso combustor, i.e., 1.5 millisecond residence time and 35 micron droplet size (32), small NO_x reductions are predicted.

Exposure time at peak temperature is the most important parameter in determining the level of NO_x emissions (see equation(6)). In the absence of engine redesign, the best way of decreasing this exposure time is to delay ignition of the fuel. Some of the antiknock compounds used in gasoline were tested as gas turbine ignition delay additives. The most effective antiknock compounds are the organo-metals, tetraethyl and tetramethyl lead. Other compounds, including aniline, some ketones and ethers are also known to be effective. As ignition delay additives for jet fuels, however, none of these proved to be effective.

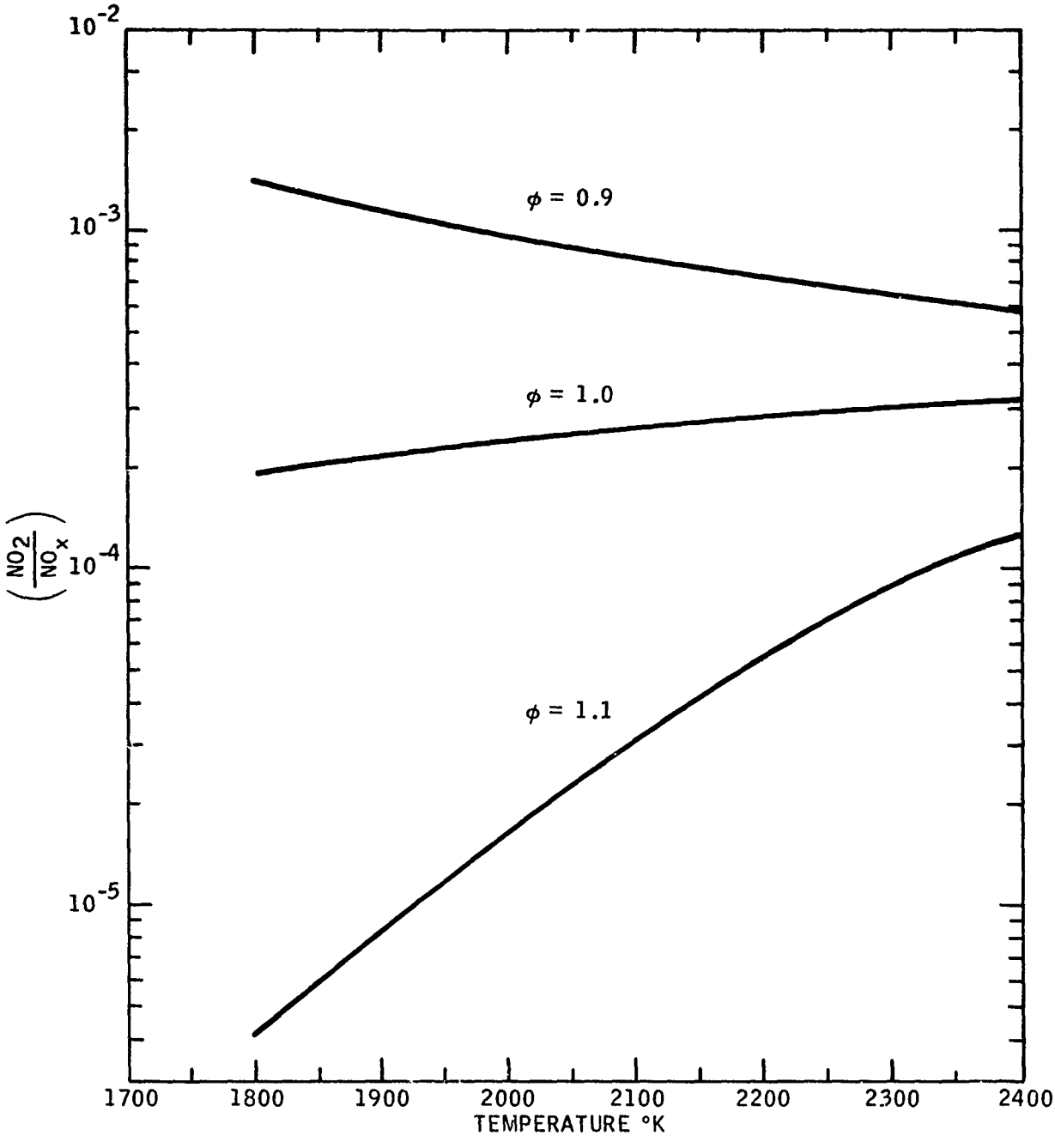

Figure 14

EFFECT OF TEMPERATURE ON NO_2/NO_x RATIO

The possibility of synergistic effects was not explored thoroughly. It was found that antimony triphenyl and carbon tetrachloride reduced NO_x in excess of the sum of the NO_x reduction values observed by the two components separately. This combination has been found effective in reducing flammability of plastics.

SECTION VI

CONCLUSIONS AND RECOMMENDATIONS

No "fully effective modification" was found. The most effective fuel modifications reduced NO_x by a third to about 4 lb NO_x per 1000 lb fuel. Other emissions and the outlet temperatures were not affected by the modifications. The effective additives contained metals in the 0.1 to 0.5% (w) range. This method of NO_x reduction will not be practicable because:

1. Metal and metal oxides emissions may be more detrimental to the environment than the NO_x that is being removed.

2. The incremental benefit in NO_x reduction may not be worth the additional fuel cost.

3. Some metals and metal oxides corrode and errode turbine blades.

4. Metals tend to catalyze the oxidation of the fuel forming sediments and deposits.

The results obtained in this program can possibly be used for NO_x reduction in aircraft during take-off and climb out. Since during take-off and climb out, both smoke and NO_x tend to be highest, one could inject ferrocene or manganese based organometallic compounds from a concentrate tank. This would help reduce smoke and NO_x during the period when these emissions are highest. However, detrimental effects on the engine may preclude the use of additives even in this case.

SECTION VII

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APPENDIX I

EXPERIMENTAL RESULTS

The experimental results are tabulated in chronological order. Table XIV reports the data in mole fraction units and Table XV reports the data in emission index units. As indicated in the Results Section, the CO_2, CO, NO_x and NO_2 values were multiplied by $(1-0.132\phi)$ in order to present the results on a wet basis. The material balance calculations were done using the formulas derived in Appendix V. The program for computing these tables is included in Appendix VII. The following notes pertain to these tables:

1. All values reported as "0" indicate that no measurement was taken.

2. A minus sign in front of C BAL or O BAL indicates that one of the components was not measured. Therefore, the value is a minimum.

3. The numerical value in front of the fuel modification symbol is percent by weight of that modification in the fuel.

4. The fuel modifications that were run as emulsions indicate the percent by weight water in front of the symbol.

5. Runs 71 to 84, 103 to 105, and 181 to 184 were reported using $(CO_2) = 12.2\phi$ rather than the measured ϕ.

6. In runs 129 and 130, ϕ's were calculated using $TE = 3351\phi + 516$ rather than the measured ϕ's.

7. The mole fraction and emission index of unburned hydrocarbon fuel, HC, is reported as methane.

8. TE is the average temperature 4.5 inches downstream from the orifice.

9. TP is the average temperature 7.5 inches downstream from the orifice. This was also the location of the probe.

10. The EI for NO_x is reported as NO_2 equivalent.

TABLE XIV

EXPERIMENTAL RESULTS - MOLE FRACTION UNITS

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
1	3.8 H2O*E	0.292	3.50	14.7	5084	55	79	0	1500	1500	50.0	98.2	-98.9
2	3.8 H2O*E	0.317	4.12	13.7	2632	4	88	0	0	0	49.0	99.0	-97.4
3	0.1 CO*NAP	0.295	3.62	0.0	1970	10	86	0	1530	1500	60.0	92.5	-27.5
4	0.1 CO*NAP	0.326	3.92	0.0	1938	8	85	0	1506	1570	61.0	90.4	-30.0
5	3.2 C6H5NH2*H	0.303	3.53	0.0	4640	15	131	0	1505	1521	57.0	94.3	-28.0
6	3.2 C6H5NH2*H	0.321	3.88	0.0	3273	9	140	0	1563	1597	58.0	93.8	-30.0
7	3.5 EGDE*H	0.306	3.45	0.0	5364	13	83	0	1488	1506	58.0	93.2	-27.9
8	3.5 EGDE*H	0.337	3.92	0.0	3506	8	87	0	1572	1608	57.0	90.8	-30.7
9	2.7 C6H6*H	0.292	3.57	0.0	3054	10	79	0	1517	1520	58.0	94.8	-27.4
10	2.7 C6H6*H	0.319	4.05	0.0	2288	14	89	0	1611	1616	59.0	96.0	-30.5
11	3.8 H2O+CH3OH*E	0.272	3.56	13.3	0	16	81	0	1510	1516	50.0	-93.4	-90.4
12	3.8 H2O+CH3OH*E	0.293	3.97	12.4	0	14	86	0	1537	1542	45.0	-96.8	-88.8
13	5.0 CCL4*H	0.301	3.52	14.2	3696	22	84	0	1483	1510	56.0	92.4	-96.6
14	5.0 CCL4*H	0.333	4.04	13.2	2151	14	94	0	1603	1623	54.0	91.6	-95.1
15	3.8 H2O+NH4CHO2*E	0.266	3.45	14.7	3721	4	75	0	1472	1488	47.0	102.5	-97.4
16	0.5 CO*NAP	0.300	3.50	14.5	4584	0	59	0	1503	1513	58.0	-94.3	-98.1
17	0.5 CO*NAP	0.333	4.06	13.3	3752	0	64	0	1590	1603	57.0	-95.4	-96.1
18	3.7 C3H7NO3*H	0.288	3.46	14.0	2790	14	117	0	1463	1503	58.0	92.8	-94.6
19	3.7 C3H7NO3*H	0.333	4.13	12.8	2055	16	141	0	1623	1627	56.0	93.3	-93.6
20	0.1 CO*ACAC	0.307	3.51	13.2	2736	14	72	0	1493	1496	49.0	88.2	-91.7
21	2.5 C2H5OH*H	0.292	3.54	14.3	2886	25	78	12	1496	1500	49.0	93.7	96.6
22	2.5 C2H5OH*H	0.322	4.17	13.4	2251	20	87	13	1600	1593	50.0	97.8	96.2
23	2.5 C2H5OH*H	0.290	3.49	13.9	2621	20	80	13	1470	1493	49.0	92.5	94.3
24	3.8 H2O+NH4NO3*E	0.289	3.46	13.7	2309	12	88	13	1537	1530	47.0	91.3	93.1

TABLE XIV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
25	0.5 PB*NAP	0.304	3.46	15.3	4512	46	83	15	1453	1460	47.0	92.1	102.0
26	0.5 PB*NAP	0.336	3.92	14.2	3106	20	84	15	0	0	49.0	90.3	99.7
27	0.5 CU*NAP	0.311	3.55	15.1	2421	18	72	15	1467	1462	50.0	87.3	101.2
28	0.2 CU*NAP	0.304	3.53	15.3	1608	20	76	17	1463	1456	50.0	86.8	101.6
29	0.2 CO*NEO	0.295	3.46	15.3	2258	48	62	14	1468	1449	48.0	89.4	101.1
30	0.2 CO*NEO	0.299	3.55	14.9	2113	51	66	15	1508	1484	49.0	90.0	99.7
31	0.2 FE*NAP	0.304	3.50	14.3	2496	24	56	10	1483	1456	47.0	88.2	96.8
32	0.2 MN*NAP	0.292	3.51	14.4	2356	20	77	13	1467	1463	47.0	91.7	96.8
33	3.8 H2O+N2H4.2C2H4O2*E	0.273	3.49	14.5	2841	12	69	13	1423	1427	45.0	98.7	96.6
34	3.8 H2O+N2H4.2C2H4O2*E	0.285	3.65	14.0	2644	16	73	13	1480	1483	46.0	98.1	95.4
35	3.8 H2O+N2H4.2C2H4O2*E	0.273	3.54	14.1	2890	14	68	13	1470	1473	45.0	100.1	94.9
36	0.1 MN*NAP	0.298	3.55	14.0	3050	164	68	13	1523	1503	47.0	92.8	95.5
37	0.2 CU*NAP	0.295	3.56	14.3	1922	24	67	13	1457	1446	48.0	90.9	96.6
38	0.1 CU*NAP	0.296	3.53	14.2	3027	18	72	13	1489	1482	48.0	92.6	96.3
39	0.1 FE*NAP	0.304	3.49	14.2	3321	37	75	12	1502	1470	48.0	90.0	96.5
40	0.1 FE*NAP	0.340	3.96	13.2	2865	28	82	19	1580	1607	49.0	89.6	95.1
41	0.1 CA*S	0.302	3.49	14.1	3840	23	79	13	1507	1485	48.0	91.8	96.0
42	0.1 CA*S	0.328	4.02	13.1	2894	24	91	18	1597	1583	50.0	94.1	94.5
43	0.1 NA*S	0.302	3.38	14.1	5017	48	60	10	1473	1471	49.0	92.0	95.8
44	0.1 NA*S	0.337	4.06	12.9	5327	20	71	14	1612	1594	50.0	97.7	94.6
45	3.1 POLY*H	0.313	3.32	14.5	6663	104	69	10	1429	1489	52.0	91.3	98.2
46	3.1 POLY*H	0.331	3.65	14.2	2725	26	78	10	1523	1530	47.0	84.9	98.1
47	0.1 AL*ACAC	0.285	3.56	14.2	2823	13	80	12	1483	1487	49.0	96.3	96.0
48	0.1 AL*ACAC	0.318	4.02	13.3	1940	16	90	13	1547	1557	50.0	94.9	94.9

TABLE XIV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
49	0.1 CA*NAP	0.304	3.53	14.4	4080	18	74	15	1490	1472	49.0	92.7	97.8
50	0.1 CA*NAP	0.327	4.09	13.5	2559	12	84	17	1603	1593	50.0	95.2	96.7
51	0.2 ZR*NEO	0.303	3.48	14.4	4160	16	77	13	1443	1470	49.0	92.0	97.6
52	0.2 ZR*NEO	0.330	4.06	13.5	2790	0	81	15	1554	1574	50.0	-94.2	96.7
53	0.2 ZR*NEO	0.311	0.00	14.4	5066	30	65	12	1476	1483	50.0	-11.7	-81.2
54	9.1 TENCEM*H	0.296	3.53	14.6	2066	12	74	15	1451	1450	48.0	90.2	98.0
55	9.1 TENCEM*H	0.327	4.07	13.6	1531	8	82	19	1600	1588	50.0	92.5	96.8
56	9.1 CEMALL*H	0.301	3.48	14.5	2953	18	74	15	1487	1491	48.0	89.7	97.7
57	9.1 CEMALL*H	0.341	4.13	13.4	2053	10	81	19	1600	1631	50.0	91.1	96.8
58	9.1 HFL*H	0.299	3.51	14.6	3338	18	75	15	1430	1493	48.0	91.9	98.3
59	9.1 HFL*H	0.331	4.16	13.4	1984	20	82	17	1605	1638	50.0	94.4	96.5
60	2.9 DCPD*H	0.300	3.54	14.6	2994	20	77	13	1454	1504	49.0	91.5	98.4
61	2.9 DCPD*H	0.332	4.16	13.4	2223	14	84	18	1598	1628	50.0	94.6	96.6
62	5.6 C3F6HOH*H	0.296	3.51	14.4	2763	20	74	14	1460	1513	48.0	91.5	97.1
63	5.6 C3F6HOH*H	0.323	4.14	13.2	1915	20	88	19	1594	1643	50.0	96.0	95.1
64	0.1 ZR*NEO	0.300	3.46	14.7	3842	40	71	12	1430	1493	48.0	91.7	98.7
65	0.2 V*NEO	0.289	3.44	14.9	3006	24	72	12	1515	1480	50.0	92.5	99.0
66	0.2 V*NEO	0.322	4.07	13.8	1676	24	82	17	1635	1597	52.0	94.3	97.6
67	0.2 ZN*NAP	0.294	3.51	14.8	3043	21	79	10	1502	1483	51.0	92.7	99.0
68	0.2 ZN*NAP	0.326	4.19	13.7	1651	18	94	18	1626	1612	53.0	95.7	97.9
69	0.5 C13NH2*H	0.328	4.16	13.8	2009	20	100	19	1485	1473	52.0	95.3	98.4
70	0.5 C13NH2*H	0.300	3.48	14.7	3217	17	82	15	1612	1603	50.0	90.6	98.7
71	3.3 H2O*E	0.286	3.48	14.0	3752	15	79	13	1528	1518	50.0	96.3	94.9
72	3.3 H2O*E	0.337	4.11	13.6	1959	13	86	19	1648	1646	52.0	91.6	97.5

TABLE XIV (Cout'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
73	5.0 H2O*E	0.292	3.56	14.5	3389	13	78	13	1530	1525	48.0	95.4	97.8
74	5.0 H2O*E	0.342	4.18	13.5	1599	13	88	20	1660	1655	51.0	91.0	97.4
75	10.0 H2O*E	0.286	3.48	14.8	3455	25	79	20	1470	1496	48.0	95.6	98.7
76	10.0 H2O*E	0.333	4.06	13.9	1920	22	89	23	1618	1617	51.0	91.5	98.5
77	20.0 H2O*E	0.288	3.51	14.5	2958	20	79	35	1487	1478	47.0	94.4	97.3
78	20.0 H2O*E	0.335	4.09	13.3	1744	18	97	38	1615	1596	48.0	91.2	95.8
79	0.33 CH3OH*E	0.284	3.46	14.2	4496	14	73	19	1513	1510	49.0	98.3	95.9
80	0.33 CH3OH*E	0.342	4.18	13.2	2125	20	92	31	1643	1640	51.0	92.1	96.1
81	0.07 H2O+NH3*E	0.286	3.48	14.6	3701	20	74	20	1502	1506	48.0	96.2	97.8
82	0.07 H2O+NH3*E	0.338	4.12	13.6	1863	13	91	33	1641	1636	51.0	91.3	97.6
83	3.5 H2O+N2H4*E	0.282	3.44	14.8	3177	18	100	31	1470	1490	49.0	95.2	98.3
84	3.5 H2O+N2H4*E	0.329	4.02	13.8	2535	28	105	38	1550	1573	47.0	93.1	97.9
85	33.0 H2O*E	0.272	3.33	15.0	4387	41	69	23	1437	1472	45.0	99.0	98.6
86	0.1 LI*NEO	0.310	3.45	14.7	6042	12	76	13	1483	1503	49.0	93.6	99.6
87	9.1 MS*H	0.306	3.50	14.7	4270	18	80	22	1490	1513	49.0	91.8	99.3
88	9.1 MS*H	0.336	4.04	13.9	2795	16	96	27	1583	1595	50.0	92.1	98.8
89	0.1 FE*ACAC	0.311	3.47	14.7	4347	28	75	20	1476	1509	49.0	89.9	99.3
90	0.1 FE*ACAC	0.336	4.04	13.9	3081	24	83	23	1580	1585	47.0	92.8	98.8
91	0.2 MN*NEO	0.295	3.46	14.9	4108	26	62	19	1497	1500	51.0	93.8	99.6
92	0.2 MN*NEO	0.329	4.06	14.0	3300	14	73	25	1593	1583	52.0	95.6	99.2
93	1.6 ARL-56	0.302	3.46	14.7	4921	24	78	15	1482	1483	48.0	93.6	99.1
94	1.6 ARL-56	0.336	3.99	13.9	3058	12	88	26	1597	1587	47.0	91.6	98.6
95	3.8 H2O*E	0.299	3.55	14.8	4394	16	81	18	1518	1520	49.0	95.4	99.7
96	3.8 H2O*E	0.328	4.07	14.0	2702	8	92	19	1611	1612	50.0	94.8	99.1

TABLE XIV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
97	3.8 H2O+B4367*E	0.292	3.49	14.9	3942	20	76	19	1487	1490	49.0	95.1	99.6
98	3.8 H2O+B4367*E	0.321	4.07	14.0	2873	12	84	24	1593	1593	50.0	97.2	98.9
99	3.8 H2O+(NH4)2M004*E	0.293	3.48	14.6	4406	23	77	18	1463	1496	49.0	95.7	98.2
100	3.8 H2O+(NH4)2M004*E	0.320	4.00	13.6	3208	24	85	19	1573	1580	46.0	96.7	96.6
101	0.1 CU*ACAC	0.310	3.52	14.6	4244	14	76	19	1513	1517	49.0	91.0	99.0
102	0.1 CU*ACAC	0.339	4.06	13.8	2674	14	86	21	1620	1620	50.0	91.5	98.5
103	0.15 CO*ACAC	0.282	3.47	14.7	5536	34	65	19	1501	1487	50.0	102.0	98.5
104	0.15 CO*ACAC	0.328	4.02	13.5	4377	22	74	25	1553	1565	46.0	97.4	96.8
105	0.2 MN*NAP	0.300	3.46	14.7	5138	90	53	10	1517	1521	48.0	94.9	99.0
106	0.2 FE*NAP	0.309	3.50	14.8	3740	32	77	29	1453	1470	48.0	89.7	99.7
107	0.13 SDMA	0.304	3.50	14.6	3431	48	74	22	1415	1463	49.0	90.5	98.5
108	0.1 LI*S	0.309	3.48	14.8	3476	30	79	13	1533	1535	49.0	88.7	99.6
109	0.1 LI*S	0.309	3.48	14.7	7097	56	66	13	1538	5113	50.0	97.1	100.0
110	0.1 LI*S	0.325	4.09	13.8	3541	22	83	27	1630	1625	52.0	98.0	98.3
111	3.1 POLY*H	0.309	3.50	14.8	3980	18	82	21	1535	1532	50.0	90.3	99.8
112	3.1 POLY*H	0.333	4.14	13.9	2032	34	96	22	1635	1632	51.0	93.5	99.0
113	0.1 CU*NAP	0.318	3.46	14.7	4502	24	74	18	1542	1538	51.0	88.0	99.6
114	0.1 FE*NAP	0.311	0.00	14.6	4603	18	73	17	1545	1533	51.0	-10.6	-82.0
115	0.1 FE*NAP	0.325	0.00	13.8	2320	20	88	26	1653	1643	53.0	-5.1	-78.1
116	3.8 H2O+NH4CHO2*E	0.298	3.53	14.6	4420	18	78	20	1560	1535	49.0	95.3	98.6
117	3.8 H2O+NH4CHO2*E	0.318	4.12	13.7	2423	14	89	23	1657	1637	48.0	98.2	97.4
118	3.8 H2O+N2H4.2C2H4O2*E	0.322	3.49	14.8	4235	20	74	19	1533	1517	50.0	87.0	100.3
119	0.1 BA*S	0.310	3.52	14.7	5250	22	77	19	1530	1502	48.0	93.4	99.7
120	0.1 BA*S	0.333	4.14	13.8	2414	12	95	28	1633	1623	50.0	94.3	98.6

TABLE XI" (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
121	0.1 MN*CI2	0.310	3.50	14.6	4052	14	66	18	1488	1455	50.0	90.1	98.9
122	0.1 MN*CI2	0.333	4.08	13.6	3220	14	78	26	1629	1584	52.0	94.7	97.5
123	0.1 NA*S	0.298	3.56	14.7	6174	18	64	19	1542	1508	51.0	100.2	99.7
124	0.1 NA*S	0.309	4.10	13.7	5083	10	77	27	1610	1571	52.0	106.7	97.6
125	0.1 NI*ACAC	0.300	3.41	15.0	4345	14	69	20	1492	1473	48.0	91.6	100.1
126	3.3 H20+CH3OH+NH3*E	0.286	3.46	15.0	3439	18	71	21	1595	1588	49.0	95.0	99.6
127	3.3 H20+CH3OH+NH3*E	0.312	3.64	14.4	2350	0	79	25	1637	1670	45.0	-88.8	98.2
128	3.0 H20+NAOH*E	0.302	3.72	14.2	6144	0	66	23	1548	1566	48.0	-102.6	98.2
129	0.1 MONEL*ACAC	0.309	3.43	14.3	5104	12	73	19	1550	1570	50.0	91.2	97.3
130	0.1 MONEL*ACAC	0.339	4.07	13.5	2451	8	90	31	1667	1630	49.0	91.2	97.0
131	3.0 H20+RBOH*E	0.314	3.50	12.7	6347	30	70	19	1523	1505	50.0	94.3	90.3
132	3.0 H20+RBOH*E	0.324	4.12	11.9	3350	8	86	27	1633	1633	48.0	98.5	89.1
133	5.8 H20+CSOH*E	0.306	3.53	13.9	7248	36	69	23	1468	1481	48.0	99.5	96.2
134	5.8 H20+CSOH*E	0.327	4.18	13.2	4091	24	84	30	C	0	46.0	100.5	96.0
135	0.1 SB*3C6H5	0.303	3.53	15.0	4848	16	76	21	1518	1511	50.0	94.8	100.9
136	0.1 SB*3C6H5	0.328	4.16	14.1	3278	8	84	27	1618	1631	52.0	98.0	100.1
137	0.1 FE*FERROCENE	0.307	3.55	15.1	6000	12	63	19	1527	1528	51.0	96.7	101.9
138	0.1 FE*FERROCENE	0.323	4.19	14.2	3182	10	74	27	1607	1637	53.0	99.9	100.6
139	5.8 H20+KOH*E	0.296	3.51	14.5	5286	48	73	19	1482	1490	50.0	97.6	98.2
140	5.8 H20+KOH*E	0.313	4.20	13.2	4651	10	82	23	1605	1622	52.0	106.7	95.7
141	0.55 TMA*H	0.306	3.53	14.9	4056	30	104	23	1525	1553	48.0	92.0	100.3
142	0.55 TMA*H	0.329	4.14	13.9	1818	18	115	32	1640	1662	49.0	94.1	98.8
143	0.1 CU*PHOS	0.303	3.46	14.8	6216	18	70	19	1515	1525	48.0	96.4	100.0
144	0.1 CU*PHOS	0.322	4.09	13.8	3253	10	79	26	1600	1623	49.5	98.2	98.5

TABLE XIV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TF F	P PSIG	C BAL PCT	O BAL PCT
145	5.8 H2O+LIOH*E	0.290	3.51	15.0	5219	32	73	17	1506	1503	47.5	99.4	100.7
146	5.8 H2O+LIOH*E	0.312	4.08	14.1	3476	10	83	23	1595	1597	49.0	101.5	99.6
147	0.1 SB+5.0 CCL4	0.294	3.48	14.9	6487	70	68	19	1508	1513	47.5	100.5	100.2
148	0.1 SB+5.0 CCL4	0.327	4.09	14.0	3373	12	78	19	1608	1612	49.5	97.0	99.6
149	0.18 PB*TEL	0.299	3.48	15.0	6792	58	72	16	1495	1492	49.0	99.6	101.1
150	0.18 PB*TEL	0.327	4.07	14.1	3900	12	83	19	1600	1609	50.5	97.7	99.9
151	0.1 CE*NAP	0.299	3.48	15.0	5184	26	77	19	0	1495	48.0	95.6	100.7
152	0.1 CE*NAP	0.322	4.12	14.1	2943	8	88	24	1612	1623	50.0	98.2	99.7
153	0.1 NI*NAP	0.294	3.53	15.0	4300	20	72	17	1500	1498	48.0	96.3	100.6
154	0.1 NI*NAP	0.315	4.14	14.2	2778	10	85	20	1605	1602	49.5	100.4	100.3
155	2.6 C4H9SH*H	0.294	3.53	15.0	5718	34	71	13	0	1485	49.0	99.8	100.9
156	2.6 C4H9SH*H	0.316	4.10	14.1	3568	16	75	11	0	1592	50.0	101.0	99.6
157	0.1 FE*NAP	0.285	3.54	15.0	3463	14	73	19	1508	1503	49.0	97.4	100.0
158	0.1 FE*NAP	0.313	4.05	14.1	2038	6	82	22	1610	1603	51.0	97.2	98.9
159	0.1 FE*NAP	0.285	3.51	14.9	3199	8	70	18	1516	1502	49.5	96.0	99.5
160	0.1 FE*NAP	0.313	4.05	13.8	2373	4	84	23	1621	1608	50.5	98.0	97.7
161	0.1 CR*NAP	0.290	3.46	15.2	4425	14	70	20	1517	1493	50.0	96.2	101.2
162	0.1 CR*NAP	0.324	4.07	14.2	2584	8	82	23	1625	1612	51.0	95.7	99.9
163	0.1 FE*FERROCENE	0.298	3.51	14.9	3075	16	60	15	1530	1510	50.0	91.6	99.9
164	0.1 FE*FERROCENE	0.328	4.09	13.9	2823	8	71	22	1645	1633	48.0	95.5	98.8
165	0.1 FE*FERROCENE	0.299	3.48	14.8	4416	16	61	16	1520	1505	50.5	93.8	99.6
166	0.1 FE*FERROCENE	0.330	4.09	13.9	3035	10	72	22	1640	1608	49.0	95.4	98.9
167	0.1 CO*NAP	0.298	3.51	14.9	3628	14	64	17	1548	1525	49.0	92.9	100.2
168	0.1 CO*NAP	0.317	4.05	14.2	2108	10	76	21	1660	1617	50.5	96.2	99.5

TABLE XIV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
169	0.1 CO*NAP	0.294	3.53	14.9	3436	12	65	17	1533	1505	50.5	94.2	99.9
170	0.1 CO*NAP	0.317	4.12	14.0	2108	8	77	21	1650	1618	52.0	97.8	99.1
171	0.1 MN*CI2	0.292	3.51	15.0	4156	0	72	17	0	1510	49.0	-96.0	100.4
172	0.1 MN*CI2	0.306	4.08	14.2	2496	0	86	21	0	1610	48.0	-101.2	99.3
173	0.1 MN*CI2	0.301	3.50	14.9	4032	0	75	17	0	1520	50.5	-92.7	100.1
174	0.1 MN*CI2	0.313	4.08	14.1	2493	0	85	21	0	1620	48.0	-99.0	99.2
175	0.5 MN*CI2	0.293	3.53	15.1	7328	62	55	15	0	1498	48.0	104.1	102.0
176	0.5 MN*CI2	0.318	4.07	14.3	3688	34	67	16	0	1607	48.0	100.0	100.5
177	0.5 FE*FERROCENE	0.304	3.50	15.2	7008	30	64	16	0	1498	48.5	98.9	102.6
178	0.5 FE*FERROCENE	0.328	4.07	14.1	3780	20	72	18	0	1600	48.5	97.2	99.9
179	0.1 MN*NAP	0.295	3.51	15.1	5693	0	66	16	1475	1497	49.0	-98.8	101.6
180	0.1 MN*NAP	0.326	3.45	15.0	3589	0	74	21	1545	1577	48.0	-83.7	101.5
181	3.8 H20+N2H4.2C2H402*E	0.282	3.45	15.0	3711	10	83	20	0	0	49.0	96.8	99.9
182	3.8 H20+N2H4.2C2H402*E	0.335	4.09	14.1	2188	4	90	23	0	0	45.0	92.2	100.0
183	3.8 H20+N2H4.2C2H402*E	0.284	3.47	15.0	4218	60	74	16	1438	0	47.5	98.0	100.1
184	3.8 H20+N2H4.2C2H402*E	0.290	3.54	15.0	2862	16	77	19	1492	1495	46.5	94.3	100.0

TABLE XV

EXPERIMENTAL RESULTS - EMISSION INDEX UNITS

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
1	3.8 H2O*E	0.292	2726.	8328.	252.0	1.55	6.43	0.00	1500	1500	50.0	98.2	-98.9
2	3.8 H2O*E	0.317	2961.	7161.	120.3	0.10	6.61	0.00	0	0	49.0	99.0	-97.4
3	0.1 CO*NAP	0.295	2791.	0.	96.6	0.28	6.93	0.00	1530	1500	60.0	92.5	-27.5
4	0.1 CO*NAP	0.326	2741.	0.	86.2	0.20	6.21	0.00	1606	1570	61.0	90.4	-30.0
5	3.2 C6H5NH2*H	0.303	2652.	0.	221.8	0.40	10.28	0.00	1505	1521	57.0	94.3	-28.0
6	3.2 C6H5NH2*H	0.321	2754.	0.	147.8	0.23	10.39	0.00	1563	1597	58.0	93.8	-30.0
7	3.5 EGDE*H	0.306	2567.	0.	253.9	0.35	6.45	0.00	1488	1506	58.0	93.2	-27.9
8	3.5 EGDE*H	0.337	2653.	0.	151.0	0.19	6.15	0.00	1572	1608	57.0	90.8	-30.7
9	2.7 C6H6*H	0.292	2781.	0.	151.3	0.28	6.43	0.00	1517	1520	58.0	94.8	-27.4
10	2.7 C6H6*H	0.319	2893.	0.	104.0	0.36	6.64	0.00	1611	1616	59.0	96.0	-30.5
11	3.8 H2O+CH3OH*E	0.272	2973.	8078.	0.0	0.48	7.07	0.00	1510	1516	50.0	-93.4	-90.4
12	3.8 H2O+CH3OH*E	0.293	3082.	7001.	0.0	0.39	6.98	0.00	1537	1542	45.0	-96.8	-88.8
13	5.0 CCL4*H	0.301	2661.	7809.	177.8	0.60	6.64	0.00	1483	1510	56.0	92.4	-96.6
14	5.0 CCL4*H	0.333	2767.	6575.	93.7	0.34	6.73	0.00	1603	1623	54.0	91.6	-95.1
15	3.8 H2O+NH4CHO2*E	0.266	2945.	9126.	202.1	0.12	6.69	0.00	1472	1488	47.0	102.5	-97.4
16	0.5 CO*NAP	0.300	2655.	8000.	221.3	0.00	4.67	0.00	1503	1513	58.0	-94.3	-98.1
17	0.5 CO*NAP	0.333	2780.	6625.	163.5	0.00	4.58	0.00	1590	1603	57.0	-95.4	-96.1
18	3.7 C3H7NO3*H	0.288	2732.	8039.	140.1	0.40	9.65	0.00	1463	1503	58.0	92.8	-94.6
19	3.7 C3H7NO3*H	0.333	2828.	6376.	89.5	0.39	10.09	0.00	1623	1627	56.0	93.3	-93.6
20	0.1 CO*ACAC	0.307	2603.	7120.	129.1	0.37	5.58	0.00	1493	1496	49.0	88.2	-91.7
21	2.5 C2H5OH*H	0.292	2757.	8101.	143.0	0.70	6.35	0.97	1496	1300	49.0	93.7	96.6
22	2.5 C2H5OH*H	0.322	2951.	6898.	101.3	0.51	6.43	0.96	1600	1593	50.0	97.8	96.3
23	2.5 C2H5OH*H	0.290	2737.	7928.	130.8	0.57	6.55	1.06	1470	1493	49.0	92.5	94.3
24	3.8 H2O+NH4NO3*E	0.289	2722.	7840.	115.6	0.34	7.23	1.06	1537	1530	47.0	91.3	93.1

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS PER 1000 POUNDS OF FUEL	EIO2	EICO	EIHC	EINOX	EINO2	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
25	0.5 PB*NAP	0.304	2591.	8332.	215.0	1.25	6.49	1.17	1453	1460	47.0	92.1	102.0
26	0.5 PB*NAP	0.336	2661.	7011.	134.2	0.49	5.96	1.06	0	0	49.0	90.3	99.7
27	0.5 CU*NAP	0.311	2599.	8042.	112.8	0.47	5.51	1.14	1467	1462	50.0	87.3	101.2
28	0.2 CU*NAP	0.304	2643.	8332.	76.6	0.54	5.95	1.33	1463	1456	50.0	86.8	101.6
29	0.2 CO*NEO	0.295	2668.	8581.	110.8	1.34	4.99	1.12	1468	1449	48.0	89.4	101.1
30	0.2 CO*NEO	0.299	2702.	8247.	102.3	1.41	5.25	1.19	1508	1484	49.0	90.0	99.7
31	0.2 FE*NAP	0.304	2621.	7788.	118.9	0.65	4.38	0.78	1483	1456	47.0	88.2	96.8
32	0.2 MN*NAP	0.292	2734.	8158.	116.7	0.56	6.27	1.05	1467	1463	47.0	91.7	96.8
33	3.8 H2O+N2H4.2C2H4O2*E	0.273	2904.	8775.	150.4	0.36	6.00	1.13	1423	1427	45.0	98.7	96.6
34	3.8 H2O+N2H4.2C2H4O2*E	0.285	2911.	8122.	134.2	0.46	6.08	1.08	1480	1483	46.0	98.1	95.4
35	3.8 H2O+N2H4.2C2H4O2*E	0.273	2945.	8533.	153.0	0.42	5.91	1.13	1470	1473	45.0	100.1	94.9
36	0.1 MN*NAP	0.298	2710.	7775.	148.2	4.55	5.42	1.03	1523	1503	47.0	92.8	95.5
37	0.2 CU*NAP	0.295	2745.	8021.	94.3	0.67	5.40	1.04	1457	1446	48.0	90.9	96.6
38	0.1 CU*NAP	0.296	2713.	7938.	148.0	0.50	5.78	1.04	1489	1472	48.0	92.6	96.3
39	0.1 FE*NAP	0.304	2613.	7733.	158.2	1.00	5.87	0.93	1502	1470	48.0	90.0	96.5
40	0.1 FE*NAP	0.340	2657.	6443.	122.3	0.68	5.75	1.33	1580	1607	49.0	89.6	95.1
41	0.1 CA*S	0.302	2630.	7729.	184.1	0.63	6.22	1.02	1507	1485	48.0	91.8	96.0
42	0.1 CA*S	0.328	2794.	6623.	128.0	0.60	6.61	1.30	1597	1583	50.0	94.1	94.5
43	0.1 NA*S	0.302	2547.	7729.	240.6	1.31	4.72	0.78	1473	1471	49.0	92.0	95.8
44	0.1 NA*S	0.337	2748.	6351.	229.4	0.49	5.02	0.99	1612	1594	50.0	97.7	94.6
45	3.1 POLY*H	0.313	2416.	7674.	308.5	2.75	5.24	0.76	1429	1489	52.0	91.3	98.2
46	3.1 POLY*H	0.331	2514.	7115.	119.4	0.65	5.61	0.72	1523	1530	47.0	84.9	98.1
47	0.1 AL*ACAC	0.285	2840.	8238.	143.3	0.37	6.67	1.00	1483	1487	49.0	96.3	96.0
48	0.1 AL*ACAC	0.318	2880.	6931.	88.4	0.41	6.74	0.97	1547	1557	50.0	94.9	94.9

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
49	0.1 CA*NAP	0.304	2643.	7842.	194.4	0.49	5.79	1.17	1490	1472	49.0	92.7	97.8
50	0.1 CA*NAP	0.327	2851.	6845.	113.5	0.30	6.12	1.23	1603	1593	50.0	95.2	96.7
51	0.2 ZR*NEO	0.303	2614.	7868.	198.8	0.43	6.04	1.02	1443	1470	49.0	92.0	97.6
52	0.2 ZR*NEO	0.330	2805.	6784.	122.6	0.00	6.57	1.08	1554	1574	50.0	-94.2	96.7
53	0.2 ZR*NEO	0.311	0.	7669.	236.0	0.79	4.97	0.91	1476	1483	50.0	-11.7	-81.2
54	9.1 TENCEM*H	0.296	2713.	8162.	101.0	0.33	5.94	1.20	1451	1450	48.0	90.2	98.0
55	9.1 TENCEM*H	0.327	2837.	6896.	67.9	0.20	5.97	1.38	1600	1588	50.0	92.5	96.8
56	9.1 CEMALL*H	0.301	2631.	7974.	142.0	0.49	5.85	1.18	1487	1491	48.0	89.7	97.7
57	9.1 CEMALL*H	0.341	2763.	6522.	87.4	0.24	5.66	1.32	1600	1631	50.0	91.1	96.8
58	9.1 HFL*H	0.299	2671.	8081.	161.6	0.49	5.96	1.19	1430	1493	48.0	91.9	98.3
59	9.1 HFL*H	0.331	2866.	6714.	86.9	0.50	5.90	1.22	1605	1638	50.0	94.4	96.5
60	2.9 DCPD*H	0.300	2685.	8055.	144.5	0.55	6.10	1.03	1454	1504	49.0	91.5	98.4
61	2.9 DCPD*H	0.332	2857.	6694.	97.1	0.34	6.03	1.29	1598	1628	50.0	94.6	96.6
62	5.6 C3F6HOH*H	0.296	2698.	8050.	135.1	0.55	5.94	1.12	1460	1513	48.0	91.5	97.1
63	5.6 C3F6HO- *H	0.323	2921.	6774.	85.9	0.51	6.49	1.40	1594	1643	50.0	96.0	95.1
64	0.1 ZR*NEO	0.300	2624.	8110.	185.4	1.10	5.63	0.95	1430	1493	48.0	91.7	98.7
65	0.2 V*NEO	0.289	2707.	8527.	150.5	0.68	5.92	0.98	1515	1480	50.0	92.5	99.0
66	0.2 V*NEO	0.322	2880.	7104.	75.4	0.61	6.06	1.25	1635	1597	52.0	94.3	97.6
67	0.2 ZN*NAP	0.294	2716.	8329.	149.8	0.59	6.39	0.80	1502	1483	51.0	92.7	99.0
68	0.2 ZN*NAP	0.326	2930.	6967.	73.4	0.45	6.87	1.31	1626	1612	53.0	95.7	97.9
69	0.5 C13NH2*H	0.328	2891.	6976.	88.8	0.50	7.26	1.38	1485	1473	52.0	95.3	98.4
70	0.5 C13NH2*H	0.300	2640.	8110.	155.3	0.46	6.50	1.18	1612	1603	50.0	90.6	98.7
71	3.3 H20*E	0.286	2766.	8095.	189.8	0.43	6.56	1.08	1528	1518	50.0	96.3	94.9
72	3.3 H20*E	0.337	2782.	6696.	84.3	0.32	6.08	1.34	1648	1646	52.0	91.6	97.5

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2	EIO2	EICO	EIHC	EINOX	EINO2	TE	TP	P	C BAL	O BAL
			POUNDS PER 1000 POUNDS OF FUEL						F	F	PSIG	PCT	PCT
73	5.0 H20*E	0.292	2773.	8215.	168.0	0.36	6.35	1.05	1530	1525	48.0	95.4	97.8
74	5.0 H20*E	0.342	2789.	6551.	67.9	0.31	6.13	1.39	1660	1655	51.0	91.0	97.4
75	10.0 H20*E	0.286	2766.	8557.	174.8	0.72	6.56	1.66	1470	1496	48.0	95.6	98.7
76	10.0 H20*E	0.333	2780.	6924.	83.6	0.54	6.37	1.64	1618	1617	51.0	91.5	98.5
77	20.0 H20*E	0.288	2771.	8327.	148.6	0.57	6.52	2.88	1487	1478	47.0	94.4	97.3
78	20.0 H20*E	0.335	2785.	6586.	75.5	0.44	6.90	2.70	1615	1596	48.0	91.2	95.8
79	0.33 CH3OH*E	0.284	2769.	8267.	229.0	0.40	6.10	1.59	1513	1510	49.0	98.3	95.9
80	0.33 CH3OH*E	0.342	2789.	6406.	90.2	0.48	6.41	2.16	1643	1640	51.0	92.1	96.1
81	0.07 H20+NH3*E	0.286	2766.	8441.	187.2	0.57	6.15	1.66	1502	1506	48.0	96.2	97.8
82	0.07 H20+NH3*E	0.338	2781.	6676.	80.0	0.31	6.42	2.32	1641	1636	51.0	91.3	97.6
83	3.5 H20+N2H4*E	0.282	2773.	8676.	162.9	0.52	8.42	2.61	1470	1490	49.0	95.2	98.3
84	3.5 H20+N2H4*E	0.329	2786.	6956.	111.8	0.70	7.60	2.75	1550	1573	47.0	93.1	97.9
85	33.0 H20*E	0.272	2781.	9111.	233.1	1.24	6.02	2.00	1437	1472	45.0	99.0	98.6
86	0.1 LI*NEO	0.310	2534.	7854.	282.4	0.32	5.83	0.99	1483	1503	49.0	93.6	99.6
87	9.1 MS*H	0.306	2604.	7954.	202.1	0.48	6.22	1.71	1490	1513	49.0	91.8	99.3
88	9.1 MS*H	0.336	2743.	6863.	120.7	0.39	6.81	1.91	1583	1595	50.0	92.1	98.8
89	0.1 FE*ACAC	0.311	2541.	7829.	202.5	0.74	5.74	1.53	1476	1509	49.0	89.9	99.3
90	0.1 FE*ACAC	0.336	2743.	6863.	133.1	0.59	5.89	1.63	1580	1585	47.0	92.8	98.8
91	0.2 MN*NEO	0.295	2668.	8357.	201.6	0.72	4.99	1.53	1497	1500	51.0	93.8	99.6
92	0.2 MN*NEO	0.329	2813.	7057.	145.5	0.35	5.28	1.81	1593	1583	52.0	95.6	99.2
93	1.6 ARL-56	0.302	2607.	8057.	236.0	0.65	6.14	1.18	1482	1483	48.0	93.6	99.1
94	1.6 ARL-56	0.336	2709.	6863.	132.1	0.29	6.24	1.84	1597	1587	47.0	91.6	98.6
95	3.8 H20*E	0.299	2702.	8192.	212.8	0.44	6.44	1.43	1518	1520	49.0	95.4	99.7
96	3.8 H20*E	0.328	2829.	7078.	119.5	0.20	6.68	1.38	1611	1612	50.0	94.8	99.1

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS PER 1000 POUNDS OF FUEL	EIO2	EICO	EIHC	EINOX	EINO2	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
97	3.8 H2O+B4367*E	0.292	2718.	8441.	195.4	0.56	6.18	1.54	1487	1490	49.0	95.1	99.6
98	3.8 H2O+B4367*E	0.321	2889.	7229.	129.8	0.30	6.23	1.78	1593	1593	50.0	97.2	98.9
99	3.8 H2O+(NH4)2M004*E	0.293	2701.	8244.	217.6	0.64	6.25	1.46	1463	1496	49.0	95.7	98.2
100	3.8 H2O+(NH4)2M004*E	0.320	2848.	7044.	145.3	0.62	6.32	1.41	1573	1580	46.0	96.7	96.6
101	0.1 CU*ACAC	0.310	2586.	7800.	198.4	0.37	5.83	1.45	1513	1517	49.0	91.0	99.0
102	0.1 CU*ACAC	0.339	2732.	6755.	114.5	0.34	6.05	1.47	1620	1620	50.0	91.5	98.5
103	0.15 CO*ACAC	0.282	2797.	8618.	283.9	0.99	5.47	1.60	1501	1487	50.0	102.0	98.5
104	0.15 CO*ACAC	0.328	2794.	6825.	193.6	0.55	5.37	1.81	1553	1565	46.0	97.4	96.8
105	0.2 MN*NAP	0.300	2624.	8110.	248.0	2.48	4.20	0.79	1517	1521	48.0	94.9	99.0
106	0.2 FE*NAP	0.309	2579.	7932.	175.4	0.85	5.93	2.23	1453	1470	48.0	89.7	99.7
107	[illegible] SDMA	0.304	2621.	7951.	163.5	1.30	5.79	1.72	1415	1463	49.0	90.5	98.5
108	0.1 LI*S	0.309	2564.	7932.	163.0	0.80	6.08	1.00	1533	1535	49.0	88.7	99.6
109	0.1 LI*S	0.309	2564.	7879.	332.8	1.50	5.08	1.00	1538	5113	50.0	97.1	100.0
110	0.1 LI*S	0.325	2868.	7039.	158.0	0.56	6.08	1.97	1630	1625	52.0	98.0	98.3
111	3.1 POLY*H	0.309	2579.	7932.	186.6	0.48	6.31	1.61	1535	1532	50.0	90.3	99.8
112	3.1 POLY*H	0.333	2835.	6924.	88.5	0.84	6.87	1.57	1635	1632	51.0	93.5	99.0
113	0.1 CU*NAP	0.318	2479.	7660.	205.2	0.62	5.54	1.34	1542	1538	51.0	88.0	99.6
114	0.1 FE*NAP	0.311	0.	7776.	214.5	0.47	5.58	1.30	1545	1533	51.0	-10.6	-82.0
115	0.1 FE*NAP	0.325	0.	7039.	103.5	0.51	6.45	1.90	1653	1643	53.0	-5.1	-78.1
116	3.8 H2O+NH4CHO2*E	0.298	2695.	8108.	214.7	0.49	6.22	1.59	1560	1535	49.0	95.3	98.6
117	3.8 H2O+NH4CHO2*E	0.318	2952.	7139.	110.4	0.36	6.66	1.72	1657	1637	48.0	98.2	97.4
118	3.8 H2O+N2H4.2C2H4O2*E	0.322	2470.	7618.	190.7	0.51	5.47	1.40	1533	1517	50.0	87.0	100.3
119	0.1 BA*S	0.310	2586.	7854.	245.4	0.58	5.91	1.45	1530	1502	48.0	93.4	99.7
120	0.1 BA*S	0.333	2835.	6874.	105.2	0.29	6.80	2.00	1633	1623	50.0	94.3	98.6

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
121	0.1 MN*CI2	0.310	2571.	7800.	189.4	0.37	5.06	1.38	1488	1455	50.0	90.1	98.9
122	0.1 MN*CI2	0.333	2794.	6774.	140.3	0.34	5.58	1.86	1629	1584	52.0	94.7	97.5
123	0.1 NA*S	0.298	2718.	8163.	300.0	0.49	5.10	1.51	1542	1508	51.0	100.2	99.7
124	0.1 NA*S	0.309	3021.	7343.	238.3	0.26	5.93	2.08	1610	1571	52.0	106.7	97.6
125	0.1 NI*ACAC	0.300	2586.	8276.	209.7	0.38	5.47	1.58	1492	1473	48.0	91.6	100.1
126	3.3 H2O+CH3OH+NH3*E	0.286	2750.	8673.	173.9	0.52	5.90	1.74	1595	1588	49.0	95.0	99.6
127	3.3 H2O+CH3OH+NH3*E	0.312	2657.	7645.	109.1	0.00	6.02	1.90	1637	1670	45.0	-88.8	98.2
128	3.0 H2O+NAOH*E	0.302	2803.	7783.	294.6	0.00	5.20	1.81	1548	1566	48.0	-102.6	98.2
129	0.1 MONEL*ACAC	0.309	2527.	7664.	239.3	0.32	5.62	1.46	1550	1570	50.0	91.2	97.3
130	0.1 MONEL*ACAC	0.339	2739.	6608.	104.9	0.19	6.33	2.18	1667	1630	49.0	91.2	97.0
131	3.0 H2O+RBOH*E	0.314	2539.	6700.	293.0	0.79	5.30	1.44	1523	1505	50.0	94.3	90.3
132	3.0 H2O+RBOH*E	0.324	2898.	6089.	149.9	0.20	6.32	1.98	1633	1633	48.0	98.5	89.1
133	5.8 H2O+CSOH*E	0.306	2626.	7521.	343.1	0.97	5.36	1.78	1468	1481	48.0	99.5	96.2
134	5.8 H2O+CSOH*E	0.327	2914.	6693.	181.5	0.60	6.12	2.18	0	0	46.0	100.5	96.0
135	0.1 SB*3C6H5	0.303	2652.	8195.	231.7	0.43	5.96	1.64	1518	1511	50.0	94.8	100.9
136	0.1 SB*3C6H5	0.328	2891.	7128.	145.0	0.20	6.10	1.96	1618	1631	52.0	98.0	100.1
137	0.1 FE*FERROCENE	0.307	2633.	8145.	283.1	0.32	4.88	1.47	1527	1528	51.0	96.7	101.9
138	0.1 FE*FERROCENE	0.323	2956.	7287.	142.8	0.25	5.45	1.99	1607	1637	53.0	99.9	100.6
139	5.8 H2O+KOH*E	0.296	2698.	8106.	258.5	1.34	5.86	1.52	1482	1490	50.0	97.6	98.2
140	5.8 H2O+KOH*E	0.313	3056.	6986.	215.3	0.26	6.23	1.74	1605	1622	52.0	106.7	95.7
141	0.55 TMA*H	0.306	2626.	8062.	192.0	0.81	8.09	1.78	1525	1553	48.0	92.0	100.3
142	0.55 TMA*H	0.329	2869.	7006.	80.1	0.45	8.33	2.31	1640	1662	49.0	94.1	98.8
143	0.1 CU*PHOS	0.303	2599.	8102.	297.1	0.49	5.49	1.49	1515	1525	48.0	96.4	100.0
144	0.1 CU*PHOS	0.322	2895.	7145.	146.5	0.25	5.84	1.92	1500	1623	49.5	98.2	98.5

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
145	5.8 H2O+LIOH*E	0.290	2752.	8590.	260.4	0.91	5.98	1.39	1506	1503	47.5	99.4	100.7
146	5.8 H2O+LIOH*E	0.312	2978.	7534.	161.4	0.26	6.33	1.75	1595	1597	49.0	101.5	99.6
147	0.1 SB+5.0 CCL4	0.294	2692.	8385.	319.4	1.96	5.50	1.53	1508	1513	47.5	100.5	100.2
148	0.1 SB+5.0 CCL4	0.327	2851.	7134.	149.6	0.30	5.68	1.38	1608	1612	49.5	97.0	99.6
149	0.18 PB*TEL	0.299	2648.	8314.	328.9	1.60	5.72	1.27	1495	1492	49.0	99.6	101.1
150	0.18 PB*TEL	0.327	2837.	7160.	173.0	0.30	6.05	1.38	1600	1609	50.5	97.7	99.9
151	0.1 CE*NAP	0.299	2648.	8314.	251.0	0.71	6.12	1.51	0	1495	48.0	95.6	100.7
152	0.1 CE*NAP	0.322	2916.	7268.	132.5	0.20	6.51	1.77	1612	1623	50.0	98.2	99.7
153	0.1 NI*NAP	0.294	2731.	8464.	211.7	0.56	5.82	1.37	1500	1498	48.0	96.3	100.6
154	0.1 NI*NAP	0.315	2994.	7505.	127.8	0.26	6.42	1.51	1605	1602	49.5	100.4	100.3
155	2.6 C4H9SH*H	0.294	2731.	8464.	281.5	0.95	5.74	1.05	0	1485	49.0	99.8	100.9
156	2.6 C4H9SH*H	0.316	2956.	7409.	163.7	0.41	5.65	0.82	0	1592	50.0	101.0	99.6
157	0.1 FE*NAP	0.285	2824.	8708.	75.8	0.40	6.08	1.58	1508	1503	49.0	97.4	100.0
158	0.1 FE*NAP	0.313	2947.	7484.	94.3	0.15	6.23	1.67	1610	1603	51.0	97.2	98.9
159	0.1 FE*NAP	0.285	2800.	8679.	162.4	0.23	5.83	1.50	1516	1502	49.5	96.0	99.5
160	0.1 FE*NAP	0.313	2947.	7335.	109.8	0.10	6.39	1.74	1621	1608	50.5	98.0	97.7
161	0.1 CR*NAP	0.290	2713.	8698.	220.8	0.39	5.73	1.63	1517	1493	50.0	96.2	101.2
162	0.1 CR*NAP	0.324	2863.	7271.	115.6	0.20	6.03	1.69	1625	1612	51.0	95.7	99.9
163	0.1 FE*FERROCENE	0.298	2680.	8297.	149.4	0.44	4.79	1.19	1530	1510	50.0	91.6	99.9
164	0.1 FE*FERROCENE	0.328	2843.	7037.	124.8	0.20	5.16	1.59	1645	1633	48.0	95.5	98.8
165	0.1 FE*FERROCENE	0.299	2648.	8209.	213.8	0.44	4.85	1.27	1520	1505	50.5	93.8	99.6
166	0.1 FE*FERROCENE	0.330	2826.	6990.	133.4	0.25	5.20	1.58	1640	1608	49.0	95.4	98.9
167	0.1 CO*NAP	0.298	2680.	8325.	176.3	0.38	5.10	1.35	1548	1525	49.0	92.9	100.2
168	0.1 CO*NAP	0.317	2911.	7433.	96.4	0.26	5.71	1.57	1660	1617	50.5	96.2	99.5

TABLE XV (Cont'd.)

RUN	FUEL MODIFICATION	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TF F	TP F	P PSIG	C BAL PCT	O BAL PCT
169	0.1 CO*NAP	0.294	2731.	8407.	169.2	0.33	5.25	1.37	1533	1505	50.5	94.2	99.9
170	0.1 CO*NAP	0.317	2961.	7360.	96.4	0.20	5.78	1.57	1650	1618	52.0	97.8	99.1
171	0.1 MN*CI2	0.292	2734.	8521.	206.0	0.00	5.86	1.38	0	1510	49.0	-96.0	100.4
172	0.1 MN*CI2	0.306	3035.	7689.	118.1	0.00	6.68	1.63	0	1610	48.0	-101.2	99.3
173	0.1 MN*CI2	0.301	2646.	8210.	194.0	0.00	5.92	1.34	0	1520	50.5	-92.7	100.1
174	0.1 MN*CI2	0.313	2969.	7484.	115.4	0.00	6.46	1.59	0	1620	48.0	-99.0	99.2
175	0.5 MN*CI2	0.293	2740.	8571.	362.0	1.75	4.46	1.21	0	1498	48.0	104.1	102.0
176	0.5 MN*CI2	0.318	2916.	7462.	168.1	0.88	5.01	1.19	0	1607	48.0	100.0	100.5
177	0.5 FE*FERROCENE	0.304	2621.	8311.	333.9	0.81	5.01	1.25	0	1498	48.5	98.9	102.6
178	0.5 FE*FERROCENE	0.328	2829.	7138.	167.2	0.50	5.23	1.30	0	1600	48.5	97.2	99.9
179	0.1 MN*NAP	0.295	2707.	8514.	279.4	0.00	5.32	1.29	1475	1497	49.0	-98.8	101.6
180	0.1 MN*NAP	0.326	2412.	7674.	159.7	0.00	5.41	1.53	1545	1577	48.0	-83.7	101.5
181	3.8 H2O+N2H4.2C2H4O2*E	0.282	2781.	8846.	190.3	0.29	6.99	1.68	0	0	49.0	96.8	99.9
182	3.8 H2O+N2H4.2C2H4O2*E	0.335	2785.	7002.	94.8	0.09	6.40	1.63	0	0	45.0	92.2	100.0
183	3.8 H2O+N2H4.2C2H4O2*E	0.284	2777.	8785.	214.8	1.74	6.19	1.33	1438	0	47.5	98.0	100.1
184	3.8 H2O+N2H4.2C2H4O2*E	0.290	2776.	8561.	142.8	0.45	6.31	1.55	1492	1495	46.5	94.3	100.0

APPENDIX II

REFERENCE EMISSIONS

The reference emissions were calculated for the equivalence ratio of the modified fuel runs and are reported in Table XVI. The appropriate least squares relationships given in Tables IX and X were used to calculate the emissions. The carbon and oxygen balances were calculated using the calculated reference emissions. The formulas used for the material balance calculations are derived in Appendix V. The program for computing these tables is included in Appendix VII. In four runs the least squares HC line predicted negative values. These were reported as zero.

TABLE XVI

REFERENCE EMISSIONS

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
1	3.8 H20*E	0.292	3.55	14.2	2924	20	83	14	1486	1501	50.0	94.1	96.3
2	3.8 H20*E	0.317	3.86	13.7	2626	66	88	15	1548	1560	49.0	93.2	96.2
3	0.1 CO*NAP	0.295	3.59	14.1	2888	26	84	14	1494	1508	60.0	94.0	96.3
4	0.1 CO*NAP	0.326	3.96	13.5	2519	82	90	16	1570	1581	61.0	92.8	96.2
5	3.2 C6H5NH2*H	0.303	3.69	14.0	2793	40	86	14	1513	1527	57.0	93.7	96.2
6	3.2 C6H5NH2*H	0.321	3.90	13.6	2578	73	89	15	1558	1569	58.0	93.0	96.2
7	3.5 EGDE*H	0.306	3.72	13.9	2757	46	86	14	1521	1534	58.0	93.6	96.2
8	3.5 EGDE*H	0.337	4.10	13.3	2387	102	92	16	1597	1607	57.0	92.5	96.1
9	2.7 C6H6*H	0.292	3.55	14.2	2924	20	83	14	1486	1501	58.0	94.1	96.3
10	2.7 C6H6*H	0.319	3.88	13.7	2602	69	88	15	1553	1565	59.0	93.1	96.2
11	3.8 H20+CH3OH*E	0.272	3.31	14.6	3162	0	80	13	1437	1453	50.0	95.1	96.3
12	3.8 H20+CH3OH*E	0.293	3.56	14.2	2912	22	84	14	1489	1503	45.0	94.1	96.3
13	5.0 CCL4*H	0.301	3.66	14.0	2817	37	85	14	1508	1522	56.0	93.8	96.2
14	5.0 CCL4*H	0.333	4.05	13.4	2435	95	91	16	1587	1598	54.0	92.6	96.1
15	3.8 H20+NH4CHO2*E	0.266	3.24	14.7	3234	0	79	12	1422	1439	47.0	95.5	96.4
16	0.5 CO*NAP	0.300	3.65	14.0	2829	35	85	14	1506	1520	58.0	93.8	96.2
17	0.5 CO*NAP	0.333	4.05	13.4	2435	95	91	16	1587	1598	57.0	92.6	96.1
18	3.7 C3H7NO3*H	0.288	3.50	14.3	2972	13	83	13	1476	1491	58.0	94.3	96.3
19	3.7 C3H7NO3*H	0.333	4.05	13.4	2435	95	91	16	1587	1598	56.0	92.6	96.1
20	0.1 CO*ACAC	0.307	3.73	13.9	2745	48	86	14	1523	1536	49.0	93.5	96.2
21	2.5 C2H5OH*H	0.292	3.55	14.2	2924	20	83	14	1486	1501	49.0	94.1	96.3
22	2.5 C2H5OH*H	0.322	3.92	13.6	2566	75	89	15	1560	1572	50.0	93.0	96.2
23	2.5 C2H5OH*H	0.290	3.53	14.2	2948	17	83	14	1481	1496	49.0	94.2	96.3
24	3.8 H20+NH4NO3*E	0.289	3.51	14.3	2960	15	83	13	1479	1493	47.0	94.3	96.3

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
25	0.5 PB*NAP	0.304	3.70	14.0	2781	42	86	14	1516	1529	47.0	93.6	96.2
26	0.5 PB*NAP	0.336	4.09	13.3	2399	100	92	16	1595	1605	49.0	92.5	96.1
27	0.5 CU*NAP	0.311	3.78	13.8	2697	55	87	15	1533	1546	50.0	93.4	96.2
28	0.2 CU*NAP	0.304	3.70	14.0	2781	42	86	14	1516	1529	50.0	93.6	96.2
29	0.2 CO*NEO	0.295	3.59	14.1	2888	26	84	14	1494	1508	48.0	94.0	96.3
30	0.2 CO*NEO	0.299	3.64	14.1	2840	33	85	14	1503	1517	49.0	93.8	96.3
31	0.2 FE*NAP	0.304	3.70	14.0	2781	42	86	14	1516	1529	47.0	93.6	96.2
32	0.2 MN*NAP	0.292	3.55	14.2	2924	20	83	14	1486	1501	47.0	94.1	96.3
33	3.8 H20+N2H4.2C2H4O2*E	0.273	3.32	14.6	3150	0	80	13	1439	1455	45.0	95.1	96.3
34	3.8 H20+N2H4.2C2H4O2*E	0.285	3.47	14.3	3007	8	82	13	1469	1484	46.0	94.5	96.3
35	3.8 H20+N2H4.2C2H4O2*E	0.273	3.32	14.6	3150	0	80	13	1439	1455	45.0	95.1	96.3
36	0.1 MN*NAP	0.298	3.62	14.1	2852	31	85	14	1501	1515	47.0	93.9	96.3
37	0.2 CU*NAP	0.295	3.59	14.1	2888	26	84	14	1494	1508	48.0	94.0	96.3
38	0.1 CU*NAP	0.296	3.60	14.1	2876	28	84	14	1496	1510	48.0	94.0	96.3
39	0.1 FE*NAP	0.304	3.70	14.0	2781	42	86	14	1516	1529	48.0	93.6	96.2
40	0.1 FE*NAP	0.340	4.14	13.2	2352	108	92	16	1604	1614	49.0	92.4	96.1
41	0.1 CA*S	0.302	3.67	14.0	2805	39	85	14	1511	1524	48.0	93.7	96.2
42	0.1 CA*S	0.328	3.99	13.5	2495	86	90	16	1575	1586	50.0	92.8	96.2
43	0.1 NA*S	0.302	3.67	14.0	2805	39	85	14	1511	1524	49.0	93.7	96.2
44	0.1 NA*S	0.337	4.10	13.3	2387	102	92	16	1597	1607	50.0	92.5	96.1
45	3.1 POLY*H	0.313	3.81	13.8	2674	59	87	15	1538	1550	52.0	93.3	96.2
46	3.1 POLY*H	0.331	4.03	13.4	2459	91	91	16	1582	1593	47.0	92.7	96.1
47	0.1 AL*ACAC	0.285	3.47	14.8	4616	23	73	16	1471	1476	49.0	98.7	99.1
48	0.1 AL*ACAC	0.318	3.88	14.2	3061	15	86	22	1581	1578	50.0	94.2	98.6

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
49	0.1 CA*NAP	0.304	3.71	14.4	3721	19	81	20	1535	1535	49.0	96.0	98.8
50	0.1 CA*NAP	0.327	3.99	14.0	2636	13	89	24	1612	1606	50.0	93.1	98.5
51	0.2 ZR*NEO	0.303	3.69	14.5	3768	19	81	20	1531	1532	49.0	96.1	98.9
52	0.2 ZR*NEO	0.330	4.02	13.9	2495	13	90	24	1622	1615	50.0	92.8	98.5
53	0.2 ZR*NEO	0.311	3.79	14.3	3391	17	84	21	1558	1557	50.0	95.1	98.7
54	9.1 TENCEM*H	0.296	3.61	14.6	4098	20	78	18	1508	1510	48.0	97.1	99.0
55	9.1 TENCEM*H	0.327	3.99	14.0	2636	13	89	24	1612	1606	50.0	93.1	98.5
56	9.1 CEMALL*H	0.301	3.67	14.5	3862	19	80	19	1524	1526	48.0	96.4	98.9
57	9.1 CEMALL*H	0.341	4.16	13.7	1976	10	94	26	1659	1649	50.0	91.6	98.3
58	9.1 HFL*H	0.299	3.64	14.5	3956	20	79	19	1518	1520	48.0	96.7	98.9
59	9.1 HFL*H	0.331	4.03	13.9	2448	13	90	25	1625	1618	50.0	92.7	98.4
60	2.9 DCPD*H	0.300	3.66	14.5	3909	19	80	19	1521	1523	49.0	96.5	98.9
61	2.9 DCPD*H	0.332	4.05	13.9	2401	12	91	25	1628	1622	50.0	92.6	98.4
62	5.6 C3F6HOH*H	0.296	3.61	14.6	4098	20	78	18	1508	1510	48.0	97.1	99.0
63	5.6 C3F6HOH*H	0.323	3.94	14.0	2825	14	88	23	1598	1594	50.0	93.6	98.6
64	0.1 ZR*NEO	0.300	3.66	14.5	3909	19	80	19	1521	1523	48.0	96.5	98.9
65	0.2 V*NEO	0.289	3.52	14.8	4428	22	76	17	1484	1489	50.0	98.1	99.1
66	0.2 V*NEO	0.322	3.92	14.1	2872	15	87	23	1595	1591	52.0	93.7	98.6
67	0.2 ZN*NAP	0.294	3.58	14.7	4192	21	78	18	1501	1504	51.0	97.4	99.0
68	0.2 ZN*NAP	0.326	3.97	14.0	2683	14	89	24	1608	1603	53.0	93.3	98.5
69	0.5 C13NH2*H	0.328	4.00	13.9	2589	13	89	24	1615	1609	52.0	93.0	98.5
70	0.5 C13NH2*H	0.300	3.66	14.5	3909	19	80	19	1521	1523	50.0	96.5	98.9
71	3.3 H2O*E	0.286	3.49	14.8	4569	23	75	17	1474	1480	50.0	98.6	99.1
72	3.3 H2O*E	0.337	4.11	13.8	2165	11	92	26	1645	1637	52.0	92.0	98.3

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
73	5.0 H20*E	0.292	3.56	14.7	4286	21	77	18	1494	1498	48.0	97.7	99.0
74	5.0 H2C*E	0.342	4.17	13.7	1929	10	94	27	1662	1652	51.0	91.5	98.3
75	10.0 H20*E	0.286	3.49	14.8	4569	23	75	17	1474	1480	48.0	98.6	99.1
76	10.0 H20*E	0.333	4.06	13.8	2353	12	91	25	1632	1625	51.0	92.5	98.4
77	20.0 H20*E	0.288	3.51	14.8	4475	22	76	17	1481	1486	47.0	98.3	99.1
78	20.0 H20*E	0.335	4.08	13.8	2259	12	92	25	1638	1631	48.0	92.2	98.4
79	0.33 CH3OH*E	0.284	3.46	14.9	4663	23	74	16	1468	1473	49.0	98.9	99.1
80	0.33 CH3OH*E	0.342	4.17	13.7	1929	10	94	27	1662	1652	51.0	91.5	98.3
81	0.07 H20+NH3*E	0.286	3.49	14.8	4569	23	75	17	1474	1480	48.0	98.6	99.1
82	0.07 H20+NH3*E	0.338	4.12	13.7	2118	11	93	26	1648	1640	51.0	91.9	98.3
83	3.5 H20+N2H4*E	0.282	3.44	14.9	4758	23	74	16	1461	1467	49.0	99.2	99.2
84	3.5 H20+N2H4*E	0.329	4.01	13.9	2542	13	90	24	1618	1612	47.0	92.9	98.5
85	33.0 H20*E	0.272	3.32	15.1	5229	26	70	14	1427	1436	45.0	100.8	99.3
86	0.1 LI*NEO	0.310	3.78	14.3	3438	17	83	21	1555	1554	49.0	95.2	98.8
87	9.1 MS*H	0.306	3.73	14.4	3626	18	82	20	1541	1541	49.0	95.7	98.8
88	9.1 MS*H	0.336	4.10	13.8	2212	11	92	25	1642	1634	50.0	92.1	98.4
89	0.1 FE*ACAC	0.311	3.79	14.3	3391	17	84	21	1558	1557	49.0	95.1	98.7
90	0.1 FE*ACAC	0.336	4.10	13.8	2212	11	92	25	1642	1634	47.0	92.1	98.4
91	0.2 MN*NEO	0.295	3.60	14.6	4145	21	78	18	1504	1507	51.0	97.2	99.0
92	0.2 MN*NEO	0.329	4.01	13.9	2542	13	90	24	1618	1612	52.0	92.9	98.5
93	1.6 ARL-56	0.302	3.68	14.5	3815	19	80	19	1528	1529	48.0	96.3	98.9
94	1.6 ARL-56	0.336	4.10	13.8	2212	11	92	25	1642	1634	47.0	92.1	98.4
95	3.8 H20*E	0.299	3.64	14.5	3956	20	79	19	1518	1520	49.0	96.7	98.9
96	3.8 H20*E	0.328	4.00	13.9	2589	13	89	24	1615	1609	50.0	93.0	98.5

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
97	3.8 H20+B4367*E	0.292	3.56	14.7	4286	21	77	18	1494	1498	49.0	97.7	99.0
98	3.8 H20+B4367*E	0.321	3.91	14.1	2919	15	87	23	1591	1588	50.0	93.8	98.6
99	3.8 H20+(NH4)2M004*E	0.293	3.57	14.7	4239	21	77	18	1498	1501	49.0	97.5	99.0
100	3.8 H20+(NH4)2M004*E	0.320	3.90	14.1	2966	15	87	23	1588	1585	46.0	94.0	98.6
101	0.1 CU*ACAC	0.310	3.78	14.3	3438	17	83	21	1555	1554	49.0	95.2	98.8
102	0.1 CU*ACAC	0.339	4.13	13.7	2071	11	93	26	1652	1643	50.0	91.8	98.3
103	0.15 CO*ACAC	0.282	3.44	14.9	4758	23	74	16	1461	1467	50.0	99.2	99.2
104	0.15 CO*ACAC	0.328	4.00	13.9	2589	13	89	24	1615	1609	46.0	93.0	98.5
105	0.2 MN*NAP	0.300	3.66	14.5	3909	19	80	19	1521	1523	48.0	96.5	98.9
106	0.2 FE*NAP	0.309	3.77	14.3	3485	17	83	21	1551	1551	48.0	95.3	98.8
107	0.13 SDMA	0.304	3.71	14.4	3721	19	81	20	1535	1535	49.0	96.0	98.8
108	0.1 LI*S	0.309	3.77	14.3	3485	17	83	21	1551	1551	49.0	95.3	98.8
109	0.1 LI*S	0.309	3.77	14.3	3485	17	83	21	1551	1551	50.0	95.3	98.8
110	0.1 LI*S	0.325	3.96	14.0	2731	14	88	23	1605	1600	52.0	93.4	98.5
111	3.1 POLY*H	0.309	3.77	14.3	3485	17	83	21	1551	1551	50.0	95.3	98.8
112	3.1 POLY*H	0.333	4.06	13.8	2353	12	91	25	1632	1625	51.0	92.5	98.4
113	0.1 CU*NAP	0.318	3.88	14.2	3061	15	86	22	1581	1578	51.0	94.2	98.6
114	0.1 FE*NAP	0.311	3.79	14.3	3391	17	84	21	1558	1557	51.0	95.1	98.7
115	0.1 FE*NAP	0.325	3.96	14.0	2731	14	88	23	1605	1600	53.0	93.4	98.5
116	3.8 H20+NH4CHO2*E	0.298	3.63	14.6	4003	20	79	19	1514	1517	49.0	96.8	98.9
117	3.8 H20+NH4CHO2*E	0.318	3.88	14.2	3061	15	86	22	1581	1578	48.0	94.2	98.6
118	3.8 H20+N2H4.2C2H402*E	0.322	3.92	14.1	2872	15	87	23	1595	1591	50.0	93.7	98.6
119	0.1 BA*S	0.310	3.78	14.3	3438	17	83	21	1555	1554	48.0	95.2	98.8
120	0.1 BA*S	0.333	4.06	13.8	2353	12	91	25	1632	1625	50.0	92.5	98.4

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
121	0.1 MN*CI2	0.310	3.78	14.3	3438	17	83	21	1555	1554	50.0	95.2	98.3
122	0.1 MN*CI2	0.333	4.06	13.8	2353	12	91	25	1632	1625	52.0	92.5	98.4
123	0.1 NA*S	0.298	3.63	14.6	4003	20	79	19	1514	1517	51.0	96.8	98.9
124	0.1 NA*S	0.309	3.77	14.3	3485	17	83	21	1551	1551	52.0	95.3	98.8
125	0.1 NI*ACAC	0.300	3.66	14.5	3909	19	80	19	1521	1523	48.0	96.5	98.9
126	3.3 H20+CH3OH+NH3*E	0.286	3.49	14.8	4569	23	75	17	1474	1480	49.0	98.6	99.1
127	3.3 H20+CH3OH+NH3*E	0.312	3.80	14.3	3343	17	84	21	1561	1560	45.0	95.0	98.7
128	3.0 H20+NAOH*E	0.302	3.68	14.5	3815	19	80	19	1528	1529	48.0	96.3	98.9
129	0.1 MONEL*ACAC	0.309	3.77	14.3	3485	17	83	21	1551	1551	50.0	95.3	98.8
130	0.1 MONEL*ACAC	0.339	4.13	13.7	2071	11	93	26	1652	1643	49.0	91.8	98.3
131	3.0 H20+RBOH*E	0.314	3.83	14.2	3249	16	85	22	1568	1566	50.0	94.7	98.7
132	3.0 H20+RBOH*E	0.324	3.95	14.0	2778	14	88	23	1602	1597	48.0	93.5	98.5
133	5.8 H20+CSOH*E	0.306	3.73	14.4	3626	18	82	20	1541	1541	48.0	95.7	98.8
134	5.8 H20+CSOH*E	0.327	3.99	14.0	2636	13	89	24	1612	1606	46.0	93.1	98.5
135	0.1 SB*3C6H5	0.303	3.69	14.5	3768	19	81	20	1531	1532	50.0	96.1	98.9
136	0.1 SB*3C6H5	0.328	4.00	13.9	2589	13	89	24	1615	1609	52.0	93.0	98.5
137	0.1 FE*FERROCENE	0.307	3.74	14.4	3579	18	82	20	1545	1544	51.0	95.6	98.8
138	0.1 FE*FERROCENE	0.323	3.94	14.0	2825	14	88	23	1598	1594	53.0	93.6	98.6
139	5.8 H20+KOH*E	0.296	3.61	14.6	4098	20	78	18	1508	1510	50.0	97.1	99.0
140	5.8 H20+KOH*E	0.313	3.82	14.3	3296	17	84	21	1565	1563	52.0	94.8	98.7
141	0.55 TMA*H	0.306	3.73	14.4	3626	18	82	20	1541	1541	48.0	95.7	98.8
142	0.55 TMA*H	0.329	4.01	13.9	2542	13	90	24	1618	1612	49.0	92.9	98.5
143	0.1 CU*PHOS	0.303	3.69	14.5	3768	19	81	20	1531	1532	48.0	96.1	98.9
144	0.1 CU*PHOS	0.322	3.92	14.1	2872	15	87	23	1595	1591	49.5	93.7	98.6

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
145	5.8 H2O+LIOH*E	0.290	3.53	14.7	4381	22	76	17	1488	1492	47.5	98.0	99.1
146	5.8 H2O+LIOH*E	0.312	3.80	14.3	3343	17	84	21	1561	1560	49.0	95.0	98.7
147	0.1 SB+5.0 CCL4	0.294	3.58	14.7	4192	21	78	18	1501	1504	47.5	97.4	99.0
148	0.1 SB+5.0 CCL4	0.327	3.99	14.0	2636	13	89	24	1612	1606	49.5	93.1	98.5
149	0.18 PB*TEL	0.299	3.64	14.5	3956	20	79	19	1518	1520	49.0	96.7	98.9
150	0.18 PB*TEL	0.327	3.99	14.0	2636	13	89	24	1612	1606	50.5	93.1	98.5
151	0.1 CE*NAP	0.299	3.64	14.5	3956	20	79	19	1518	1520	48.0	96.7	98.9
152	0.1 CE*NAP	0.322	3.92	14.1	2872	15	87	23	1595	1591	50.0	93.7	98.6
153	0.1 NI*NAP	0.294	3.58	14.7	4192	21	78	18	1501	1504	48.0	97.4	99.0
154	0.1 NI*NAP	0.315	3.84	14.2	3202	16	85	22	1571	1569	49.5	94.6	98.7
155	2.6 C4H9SH*H	0.294	3.58	14.7	4192	21	78	18	1501	1504	49.0	97.4	99.0
156	2.6 C4H9SH*H	0.316	3.85	14.2	3155	16	85	22	1575	1572	50.0	94.5	98.7
157	0.1 FE*NAP	0.285	3.47	14.8	4616	23	75	16	1471	1476	49.0	98.7	99.1
158	0.1 FE*NAP	0.313	3.82	14.3	3296	17	84	21	1565	1563	51.0	94.8	98.7
159	0.1 FE*NAP	0.285	3.47	14.8	4616	23	75	16	1471	1476	49.5	98.7	99.1
160	0.1 FE*NAP	0.313	3.82	14.3	3296	17	84	21	1565	1563	50.5	94.8	98.7
161	0.1 CR*NAP	0.290	3.53	14.7	4381	22	76	17	1488	1492	50.0	98.0	99.1
162	0.1 CR*NAP	0.324	3.95	14.0	2778	14	88	23	1602	1597	51.0	93.5	98.5
163	0.1 FE*FERROCENE	0.298	3.63	14.6	4003	20	79	19	1514	1517	50.0	96.8	98.9
164	0.1 FE*FERROCENE	0.328	4.00	13.9	2589	13	89	24	1615	1609	48.0	93.0	98.5
165	0.1 FE*FERROCENE	0.299	3.64	14.5	3956	20	79	19	1518	1520	50.5	96.7	98.9
166	0.1 FE*FERROCENE	0.330	4.02	13.9	2495	13	90	24	1622	1615	49.0	92.8	98.5
167	0.1 CO*NAP	0.298	3.63	14.6	4003	20	79	19	1514	1517	49.0	96.8	98.9
168	0.1 CO*NAP	0.317	3.86	14.2	3108	16	86	22	1578	1575	50.5	94.3	98.6

TABLE XVI (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
169	0.1 CO*NAP	0.294	3.58	14.7	4192	21	78	18	1501	1504	50.5	97.4	99.0
170	0.1 CO*NAP	0.317	3.86	14.2	3108	16	66	22	1578	1575	52.0	94.3	98.6
171	0.1 MN*CI2	0.292	3.56	14.7	4286	21	77	18	1494	1498	49.0	97.7	99.0
172	0.1 MN*CI2	0.306	3.73	14.4	3626	18	82	20	1541	1541	48.0	95.7	98.8
173	0.1 MN*CI2	0.301	3.67	14.5	3862	19	80	19	1524	1526	50.5	96.4	98.9
174	0.1 MN*CI2	0.313	3.82	14.3	3296	17	84	21	1565	1563	48.0	94.8	98.7
175	0.5 MN*CI2	0.293	3.57	14.7	4239	21	77	18	1498	1501	48.0	97.5	99.0
176	0.5 MN*CI2	0.318	3.88	14.2	3061	15	86	22	1581	1578	48.0	94.2	98.6
177	0.5 FE*FERROCENE	0.304	3.71	14.4	3721	19	81	20	1535	1535	48.5	96.0	98.8
178	0.5 FE*FERROCENE	0.328	4.00	13.9	2589	13	89	24	1615	1609	48.5	93.0	98.5
179	0.1 MN*NAP	0.295	3.60	14.6	4145	21	78	18	1504	1507	49.0	97.2	99.0
180	0.1 MN*NAP	0.326	3.97	14.0	2683	14	89	24	1608	1603	48.0	93.3	98.5
181	3.8 H20+N2H4.2C2H402*E	0.282	3.44	14.9	4758	23	74	16	1461	1467	49.0	99.2	99.2
182	3.8 H20+N2H4.2C2H402*E	0.335	4.08	13.8	2259	12	92	25	1638	1631	45.0	92.2	98.4
183	3.8 H20+N2H4.2C2H402*E	0.284	3.46	14.9	4663	23	74	16	1468	1473	47.5	98.9	99.1
184	3.8 H20+N2H4.2C2H402*E	0.290	3.53	14.7	4381	22	76	17	1488	1492	46.5	98.0	99.1

APPENDIX III

MODIFICATION EFFECTIVENESS

The effectiveness of the fuel modifications was measured by comparing the experimental emissions containing the fuel modification with the reference emissions. The formula used was:

$$\frac{\text{(experimental emission)} - \text{(reference emission)}}{\text{(reference emission)}} \times 100 \qquad (9)$$

A negative quantity, therefore, indicates a reduction.

The experimental emissions were taken from Table XIV and the reference emissions from Table XVI. Asterisks indicate that no experimental measurements were taken. Any run which contains asterisks in one of the columns other than PHI, TE and TP has an incorrect value in the C BAL and O BAL columns. The program for computing these tables is included in Appendix VII. The results are presented in Table XVII and are independent of dilution effects. The dilution effects are factored out since the experimental and reference values are taken at the same equivalence ratio.

TABLE XVII

PERCENT CHANGE DUE TO MODIFICATION

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
1	3.8 H20*E	0.292	-1.44	3.51	73.86	163.22	-5.80	******	0.90	-0.06	4.31	2.73
2	3.8 H20*E	0.317	6.86	-0.00	0.22	-93.96	-0.57	******	******	******	6.27	1.[illegible]6
3	0.1 CO*NAP	0.295	0.90	******	-31.80	-62.03	1.87	******	2.41	-0.53	-1.61	-71.43
4	0.1 CO*NAP	0.326	-1.13	******	-23.06	-90.31	-5.74	******	2.27	-0.74	-2.63	-68.80
5	3.2 C6H5NH2*H	0.303	-4.21	******	66.12	-63.27	52.50	******	-0.58	-0.40	0.65	-70.91
6	3.2 C6H5NH2*H	0.321	-0.61	******	26.93	-87.75	56.87	******	0.32	1.74	0.84	-68.81
7	3.5 EGDE*H	0.306	-7.30	******	94.53	-71.91	-4.00	******	-2.18	-1.84	-0.39	-71.01
8	3.5 EGDE*H	0.337	-4.36	******	46.82	-92.19	-5.66	******	-1.59	0.02	-1.83	-68.06
9	2.7 C6H6*H	0.292	0.53	******	4.44	-52.14	-5.80	******	2.04	1.27	0.70	-71.54
10	2.7 C6H6*H	0.319	4.39	******	-12.08	-79.96	0.14	******	3.73	3.26	3.13	-68.29
11	3.8 H20+CH3OH*E	0.272	7.62	-8.92	******	0.0	1.07	******	5.05	4.30	-1.81	-6.17
12	3.8 H20+CH3OH*E	0.293	11.41	-12.56	******	-38.35	2.33	******	3.22	2.57	2.87	-7.76
13	5.0 CCL4*H	0.301	-3.85	1.27	31.20	-40.88	-1.79	******	-1.71	-0.81	-1.46	0.37
14	5.0 CCL4*H	0.333	-0.25	-1.34	-11.68	-85.30	2.76	******	0.97	1.55	-1.10	-1.08
15	3.8 H20+NH4CHO2*E	0.266	6.64	-0.16	15.05	0.0	-5.10	******	3.47	3.39	7.37	1.08
16	0.5 CO*NAP	0.300	-4.07	3.27	62.04	******	-30.87	******	-0.22	-0.46	0.52	1.92
17	0.5 CO*NAP	0.333	0.25	-0.59	54.05	******	-30.04	******	0.15	0.30	3.01	-0.04
18	3.7 C3H7NO3*H	0.288	-1.22	-1.97	-6.12	2.61	40.77	******	-0.94	0.78	-1.61	-1.75
19	3.7 C3H7NO3*H	0.333	1.98	-4.33	-15.63	-83.20	54.14	******	2.23	1.80	0.74	-2.64
20	0.1 CO*ACAC	0.307	-5.99	-5.04	-0.34	-70.89	-16.90	******	-2.01	-2.64	-5.70	-4.70
21	2.5 C2H5OH*H	0.292	-0.32	0.69	-1.31	19.65	-6.99	-14.57	0.63	-0.06	-0.47	0.34
22	2.5 C2H5OH*H	0.322	6.48	-1.47	-12.30	-73.43	-2.72	-17.30	2.53	1.33	5.18	0.13
23	2.5 C2H5OH*H	0.290	-1.05	-2.40	-11.10	15.81	-4.18	-6.71	-0.79	-0.21	-1.84	-2.06
24	3.8 H20+NH4NO3*E	0.289	-1.56	-3.94	-21.99	-22.36	5.64	-6.33	3.90	2.42	-3.15	-3.31

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
25	0.5 PB*NAP	0.304	-6.42	9.59	62.23	7.86	-3.59	1.93	-4.17	-4.54	-1 5	5.99
26	0.5 PB*NAP	0.336	-4.07	6.61	29.43	-80.13	-8.73	-9.09	******	******	-2.40	3.72
27	0.5 CU*NAP	0.311	-6.14	9.26	-10.26	-67.47	-17.61	-0.70	-4.33	-5.43	-6.51	5.19
28	0.2 CU*NAP	0.304	-4.52	9.59	-42.18	-53.11	-11.72	15.53	-3.51	-4.80	-7.31	5.58
29	0.2 CO*NEO	0.295	-3.56	8.19	-21.83	82.28	-26.56	-1.50	-1.74	-3.92	-4.91	5.02
30	0.2 CO*NEO	0.299	-2.38	5.96	-25.62	51.85	-22.50	3.90	0.27	-2.21	-4.10	3.58
31	0.2 FE*NAP	0.304	-5.33	2.43	-10.26	-43.73	-34.95	-32.04	-2.19	-4.80	-5.82	0.59
32	0.2 MN*NAP	0.292	-1.16	1.40	-19.43	-4.28	-8.18	-7.45	-1.32	-2.53	-2.60	0.55
33	3.8 H2O+N2H4.2C2H4O2*E	0.273	5.11	-0.57	-9.83	0.0	-14.11	0.10	-1.17	-1.98	3.83	0.27
34	3.8 H2O+N2H4.2C2H4O2*E	0.285	5.30	-?	.09	95.01	-11.58	-4.80	0.72	-0.0?	3.86	-0.93
35	3.8 H2O+N2H4.2C2H4O2*E	0.273	6.62	-	3.27	0.0	-15.35	0.10	2.0?	1.18	5.30	-1.49
36	0.1 MN*NAP	0.298	-2.05	-0.?8	6.91	416.17	-19.98	-9.60	1.44	-0.80	-1.16	-0.78
37	0.2 CU*NAP	0.295	-0.77	1.12	-33.46	.	-20.63	-8.54	-2.48	-4.11	-3.31	0.35
38	0.1 CU*NAP	0.296	-1.94	0.56	5.23	-36.05	-14.90	-8.89	-0.50	-1.88	-1.46	0.04
39	0.1 FE*NAP	0.304	-5.61	1.71	19.41	-13.25	-12.88	-18.45	-0.94	-3.88	-3.89	0.28
40	0.1 FE*NAP	0.340	-4.23	-0.29	21.80	-74.05	-11.61	13.62	-1.54	-0.49	-3.03	-1.05
41	0.1 CA*S	0.302	-4.98	0.71	36.90	-41.06	-7.84	-10.98	-0.28	-2.60	-2.06	-0.25
42	0.1 CA*S	0.328	0.77	-2.82	15.98	-72.14	0.50	12.12	1.38	-0.21	1.42	-1.72
43	0.1 NA*S	0.302	-7.98	0.71	78.86	23.00	-30.00	-31.52	-2.53	-3.52	-1.84	-0.46
44	0.1 NA*S	0.337	-0.94	-3.00	123.08	-80.48	-23.01	-15.44	0.91	-0.85	5.63	-1.58
45	3.1 POLY*H	0.313	-12.79	5.22	149.18	76.37	-21.38	-34.29	-7.11	-3.98	-2.15	2.07
46	3.1 POLY*H	0.331	-9.33	5.82	10.80	-71.62	-14.38	-38.35	-3.77	-3.98	-8.40	2.04
47	0.1 AL*ACAC	0.285	2.48	-4.29	-38.85	-43.92	6.71	-28.40	0.80	0.69	-2.45	-3.15
48	0.1 AL*ACAC	0.318	3.71	-6.02	-36.62	0.93	4.28	-42.60	-2.20	-1.38	0.74	-3.78

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
49	0.1 CA*NAP	0.304	-4.74	-0.30	9.65	-5.08	-9.20	-25.56	-2.93	-4.14	-3.43	-1.06
50	0.1 CA*NAP	0.327	2.61	-3.33	-2.95	-13.38	-6.04	-29.90	-0.56	-0.84	2.22	-1.82
51	0.2 ZR*NEO	0.303	-5.77	-0.44	10.40	-16.60	-5.12	-34.90	-5.78	-4.07	-4.30	-1.27
52	0.2 ZR*NEO	0.330	0.94	-2.90	11.81	******	0.63	-39.48	-4.19	-2.59	1.52	-1.78
53	0.2 ZR*NEO	0.311	******	0.72	49.40	72.34	-22.53	-43.92	-5.29	-4.76	-87.69	-17.76
54	9.1 TENCEM*H	0.296	-2.16	-0.06	-49.59	-42.14	-6.03	-19.88	-3.79	-4.02	-7.10	-0.97
55	9.1 TENCEM*H	0.327	2.11	-2.62	-41.94	-42.25	-8.28	-21.66	-0.74	-1.15	-0.68	-1.72
56	9.1 CEMALL*H	0.301	-5.15	-0.03	-23.54	-8.30	-8.04	-23.52	-2.48	-2.31	-6.95	-1.20
57	9.1 CEMALL*H	0.341	-0.64	-2.01	3.86	-6.92	-14.02	-28.97	-3.55	-1.14	-0.53	-1.51
58	9.1 HFL*H	0.299	-3.69	0.37	-15.64	-10.33	-5.99	-22.11	-5.81	-1.78	-4.94	-0.62
59	9.1 HFL*H	0.331	3.11	-3.48	-18.96	54.26	-9.67	-31.91	-1.25	1.18	1.86	-1.97
60	2.9 DCPD*H	0.300	-3.19	0.51	-23.42	0.75	-3.90	-33.11	-4.44	-1.26	-5.22	-0.51
61	2.9 DCPD*H	0.332	2.80	-3.33	-7.41	9.86	-7.81	-28.41	-1.89	0.37	2.20	-1.85
62	5.6 C3F6HOH*H	0.296	-2.71	-1.43	-32.58	-3.56	-6.03	-25.22	-3.19	0.15	-5.77	-1.88
63	5.6 C3F6HOH*H	0.323	5.15	-6.04	-32.22	35.67	-0.03	-19.28	-0.29	3.06	2.56	-3.51
64	0.1 ZR*NEO	0.300	-5.38	1.20	-1.73	101.50	-11.39	-38.26	-6.01	-1.98	-5.01	-0.20
65	0.2 V*NEO	0.289	-2.35	0.99	-32.11	7.65	-5.69	-31.32	2.04	-0.62	-5.72	-0.07
66	0.2 V*NEO	0.322	3.70	-1.91	-41.65	60.38	-6.48	-27.23	2.49	0.37	0.62	-0.99
67	0.2 ZN*NAP	0.294	-2.05	1.02	-27.42	-0.87	1.20	-45.55	0.04	-1.44	-4.81	0.01
68	0.2 ZN*NAP	0.326	5.45	-2.05	-38.48	27.88	5.52	-25.23	1.08	0.53	2.63	-0.62
69	0.5 C13NH2*H	0.328	4.05	-1.04	-22.42	46.72	11.43	-22.23	-8.07	-8.49	2.45	-0.08
70	0.5 C13NH2*H	0.300	-4.83	1.20	-17.71	-14.36	2.34	-22.62	5.95	5.24	-6.15	-0.20
71	3.3 H20*E	0.286	-0.17	-5.51	-17.89	-34.67	4.89	-23.25	3.62	2.57	-2.30	-4.25
72	3.3 H20*E	0.337	0.06	-1.15	-9.53	11.76	-7.36	-27.02	0.15	0.52	-0.45	-0.86

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
73	5.0 H2O*E	0.292	0.02	-1.30	-20.94	-39.89	0.81	-27.81	2.36	1.77	-2.33	-1.23
74	5.0 H2O*E	0.342	0.27	-1.13	-17.13	23.55	-6.93	-25.73	-0.14	0.13	-0.53	-0.89
75	10.0 H2O*E	0.286	-0.17	-0.11	-24.39	8.88	4.89	18.08	-0.31	1.09	-3.01	-0.41
76	10.0 H2O*E	0.333	0.03	0.43	-18.43	75.71	-2.69	-9.17	-0.86	-0.50	-1.03	0.09
77	20.0 H2O*E	0.288	-0.01	-1.86	-33.90	-11.18	3.95	102.37	0.38	-0.54	-3.93	-1.80
78	20.0 H2O*E	0.335	0.16	-3.62	-22.82	49.05	5.26	47.98	-1.45	-2.16	-1.12	-2.62
79	0.33 CH3OH*E	0.284	-0.05	-4.43	-3.60	-40.18	-2.18	14.59	3.07	2.46	-0.58	-3.27
80	0.33 CH3OH*E	0.342	0.27	-3.33	10.13	90.08	-2.70	15.12	-1.16	-0.78	0.67	-2.21
81	0.07 H2O+NH3*E	0.286	-0.17	-1.46	-19.01	-12.89	-1.74	18.08	1.86	1.76	-2.40	-1.32
82	0.07 H2O+NH3*E	0.338	0.00	-1.00	-12.05	13.93	-2.34	25.89	-0.48	-0.27	-0.66	-0.74
83	3.5 H2O+N2H4*E	0.282	0.08	-0.67	-33.23	-24.53	35.25	91.07	0.60	1.53	-4.01	-0.88
84	3.5 H2O+N2H4*E	0.329	0.24	-0.89	-0.29	108.81	16.55	54.42	-4.24	-2.46	0.21	-0.58
85	33.0 H2O*E	0.272	0.44	-0.71	-16.11	57.27	-2.13	59.27	0.65	2.46	-1.79	-0.72
86	0.1 LI*NEO	0.310	-8.70	2.67	75.74	-31.93	-9.05	-38.74	-4.63	-3.28	-1.60	0.86
87	9.1 MS*H	0.306	-6.16	2.07	17.74	-2.80	-2.66	7.29	-3.35	-1.86	-4.11	0.49
88	9.1 MS*H	0.336	-1.36	0.88	26.33	34.97	3.79	4.42	-3.60	-2.41	-0.03	0.45
89	0.1 FE*ACAC	0.311	-6.46	2.82	28.19	60.85	-10.61	-6.53	-5.29	-3.09	-5.45	0.57
90	0.1 FE*ACAC	0.336	-1.36	0.88	39.26	102.45	-10.26	-11.05	-3.78	-3.02	0.73	0.45
91	0.2 MN*NEO	0.295	-3.78	1.85	-0.90	24.04	-20.92	2.46	-0.52	-0.51	-3.54	0.63
92	0.2 MN*NEO	0.329	1.24	0.55	29.80	4.40	-18.97	1.59	-1.59	-1.84	2.90	0.74
93	1.6 ARL-56	0.302	-6.01	1.49	28.98	23.67	-3.48	-24.21	-3.02	-3.03	-2.77	0.23
94	1.6 ARL-56	0.336	-2.58	0.88	38.22	1.23	-4.86	0.55	-2.75	-2.90	-0.57	0.24
95	3.8 H2O*E	0.299	-2.59	1.74	11.05	-20.29	1.53	-6.53	-0.01	-0.00	-1.32	0.79
96	3.8 H2O*E	0.328	1.80	0.40	4.34	-41.31	2.51	-22.23	-0.27	0.15	1.91	0.63

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
97	3.8 H2O+B4367*E	0.292	-1.94	1.42	-8.04	-7.53	-1.78	5.51	-0.52	-0.56	-2.63	0.58
98	3.8 H2O+B4367*E	0.321	4.02	-0.64	-1.59	-20.98	-3.82	3.53	0.07	0.31	3.58	0.32
99	3.8 H2O+(NH4)2MO04*E	0.293	-2.56	-0.48	3.93	7.45	-0.92	-1.03	-2.34	-0.37	-1.87	-0.81
100	3.8 H2O+(NH4)2MO04*E	0.320	2.55	-3.62	8.13	55.76	-2.29	-17.40	-0.98	-0.31	2.91	-2.03
101	0.1 CU*ACAC	0.310	-6.84	1.97	23.44	-20.59	-9.05	-10.46	-2.70	-2.38	-4.42	0.25
102	0.1 CU*ACAC	0.339	-1.74	0.61	29.12	25.13	-8.04	-20.43	-1.95	-1.44	-0.33	0.19
103	0.15 CO*ACAC	0.287	0.95	-1.34	16.35	42.56	-12.09	17.11	2.72	1.32	2.84	-0.68
104	0.15 CO*ACAC	0.328	0.55	-3.19	69.02	61.39	-17.54	2.33	-3.86	-2.77	4.71	-1.71
105	0.2 MN*NAP	0.300	-5.38	1.20	31.42	353.38	-33.85	-48.55	-0.30	-0.14	-1.70	0.10
106	0.2 FE*NAP	0.309	-7.07	3.22	7.31	79.25	-7.47	37.83	-6.36	-5.22	-5.91	0.94
107	0.13 SDMA	0.304	-5.54	1.09	-7.79	153.13	-9.20	9.19	-7.81	-4.72	-5.73	-0.35
108	0.1 LI*S	0.309	-7.60	3.22	-0.27	68.05	-5.07	-38.22	-1.20	-1.03	-6.96	0.84
109	0.1 LI*S	0.309	-7.60	2.52	103.33	213.69	-20.69	-38.22	-0.88	229.67	1.85	1.25
110	0.1 LI*S	0.325	3.25	-1.48	29.66	53.87	-6.44	12.99	1.54	1.54	4.96	-0.23
111	3.1 POLY*H	0.309	-7.07	3.22	14.20	0.83	-1.46	-0.19	-1.07	-1.22	-5.28	1.04
112	3.1 POLY*H	0.333	2.00	0.43	-13.67	171.55	4.96	-13.12	0.18	0.43	1.13	0.60
113	0.1 CU*NAP	0.318	-10.74	3.87	47.08	51.39	-14.26	-20.52	-2.52	-2.58	-6.59	0.98
114	0.1 FE*NAP	0.311	******	2.12	35.74	3.40	-13.00	-20.55	-0.86	-1.55	-88.85	-16.95
115	0.1 FE*NAP	0.325	******	-1.48	-15.05	39.88	-0.80	8.81	2.97	2.66	-94.54	-20.73
116	3.8 H2O+NH4CHO2*E	0.298	-2.82	0.23	10.40	-11.31	-1.81	4.83	2.98	1.19	-1.57	-0.34
117	3.8 H2O+NH4CHO2*E	0.318	6.29	-3.20	-20.84	-11.69	3.12	1.56	4.75	3.69	4.24	-1.25
118	3.8 H2O+N2H4.2C2H4O2*E	0.322	-11.08	5.19	47.44	33.65	-15.60	-18.66	-3.90	-4.66	-7.17	1.75
119	0.1 BA*S	0.310	-6.84	2.67	52.70	24.79	-7.85	-10.46	-1.61	-3.35	-1.90	0.96
120	0.1 BA*S	0.333	2.00	-0.30	2.55	-4.16	3.87	10.58	0.06	-0.13	1.99	0.20

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
121	0.1 MN*CI2	0.310	-7.37	1.97	17.86	-20.59	-21.01	-15.17	-4.31	-6.37	-5.36	0.15
122	0.1 MN*CI2	0.333	0.52	-1.74	36.80	11.81	-14.72	2.68	-0.19	-2.53	2.43	-0.92
123	0.1 NA*S	0.298	-1.99	0.91	54.20	-11.31	-19.43	-0.41	1.79	-0.59	3.49	0.78
124	0.1 NA*S	0.309	8.86	-4.46	45.84	-43.98	-7.47	28.32	3.76	1.29	11.92	-1.18
125	0.1 NI*ACAC	0.300	-6.75	3.27	11.14	-29.47	-13.88	2.90	-1.94	-3.29	-5.12	1.21
126	3.3 H20+CH3OH+NH3*E	0.286	-0.75	1.24	-24.74	-21.60	-5.73	23.98	8.16	7.30	-3.62	0.49
127	3.3 H20+CH3OH+NH3*E	0.312	-4.29	0.86	-29.72	******	-6.23	15.87	4.82	7.04	-6.48	-0.53
128	3.0 H20+NAOH*E	0.302	1.06	-1.96	61.04	******	-18.33	16.21	1.29	2.40	6.58	-0.68
129	0.1 MONEL*ACAC	0.309	-8.93	-0.27	46.45	-32.78	-12.28	-9.70	-0.11	1.23	-4.34	-1.49
130	0.1 MONEL*ACAC	0.339	-1.50	-1.58	18.35	-28.50	-3.77	17.46	0.90	-0.83	-0.66	-1.34
131	3.0 H20+RBOH*E	0.314	-8.55	-10.78	95.32	79.20	-17.58	-13.37	-2.90	-3.92	-0.42	-8.50
132	3.0 H20+RBOH*E	0.324	4.32	-15.17	20.58	-44.90	-2.68	13.84	1.94	2.24	5.36	-9.58
133	5.8 H20+CSOH*E	0.306	-5.36	-3.48	99.85	94.40	-16.04	12.16	-4.78	-3.94	3.94	-2.64
134	5.8 H20+CSOH*E	0.327	4.87	-5.48	55.16	73.24	-6.04	23.70	******	******	7.91	-2.54
135	0.1 SB*3C6H5	0.303	-4.42	3.71	28.66	-16.60	-6.35	5.15	-0.89	-1.40	-1.38	2.07
136	0.1 SB*3C6H5	0.328	4.05	1.11	26.58	-41.31	-6.40	10.52	0.16	1.33	5.35	1.64
137	0.1 FE*FERROCENE	0.307	-5.13	5.00	67.62	-34.41	-23.66	-8.14	-1.16	-1.09	1.15	3.14
138	0.1 FE*FERROCENE	0.323	6.42	1.08	12.63	-32.17	-15.93	14.71	0.53	2.69	6.73	2.07
139	5.8 H20+KOH*E	0.296	-2.71	-0.74	28.99	131.44	-7.30	1.4[illegible]	-1.73	-1.38	0.52	-0.77
140	5.8 H20+KOH*E	0.313	10.09	-7.41	41.08	-41.05	-3.06	5.73	2.55	3.75	12.52	-3.05
141	0.55 TMA*H	0.306	-5.36	3.46	11.84	62.00	26.54	12.16	-1.08	0.73	3.90	1.50
142	0.55 TMA*H	0.329	3.24	-0.17	-28.49	34.23	27.65	30.04	1.32	3.06	1.29	0.34
143	0.1 CU*PHOS	0.303	-6.32	2.53	64.96	-6.17	-13.74	-4.86	-1.08	-0.48	0.28	1.16
144	0.1 CU*PHOS	0.322	4.21	-1.34	13.25	-33.17	-9.90	11.30	0.30	2.01	4.78	-0.07

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
145	5.8 H2O+LIOH*E	0.290	-0.70	2.22	19.13	44.98	-4.81	-3.69	1.21	0.72	1.46	1.66
146	5.8 H2O+LIOH*E	0.312	7.28	-0.61	3.95	-41.81	-1.48	6.60	2.13	2.36	6.90	0.89
147	0.1 SB+5.0 CCL4	0.294	-2.89	1.71	54.73	230.44	-12.89	3.46	0.44	0.56	3.20	1.22
148	0.1 SB+5.0 CCL4	0.327	2.61	0.75	27.92	-13.38	-12.75	-21.66	-0.25	0.34	4.15	1.12
149	0.18 PB*TEL	0.299	-4.51	3.26	71.66	188.95	-9.75	-16.91	-1.53	-1.85	3.02	2.21
150	0.18 PB*TEL	0.327	2.11	1.11	47.91	-13.38	-7.16	-21.66	-0.74	0.15	4.90	1.42
151	0.1 CE*NAP	0.299	-4.51	3.26	31.02	29.53	-3.48	-1.34	******	-1.65	-1.12	1.80
152	0.1 CE*NAP	0.322	4.97	0.36	2.46	-46.54	0.36	2.74	1.05	2.01	4.78	1.14
153	0.1 NI*NAP	0.294	-1.49	2.66	2.57	-5.59	-7.77	-7.43	-0.09	-0.44	-1.11	1.62
154	0.1 NI*NAP	0.315	7.83	0.39	-13.25	-39.46	-0.33	-9.55	2.11	2.07	6.16	1.44
155	2.6 C4H9SH*H	0.294	-1.49	2.66	36.39	60.50	-9.05	-29.21	******	-1.30	2.48	1.93
156	2.6 C4H9SH*H	0.316	6.45	-0.45	13.08	-1.82	-12.40	-50.65	******	1.24	6.93	0.95
157	0.1 FE*NAP	0.285	1.90	1.17	-24.99	-39.61	-2.63	13.37	2.50	1.77	-1.33	0.88
158	0.1 FE*NAP	0.313	6.16	-0.81	-38.18	-64.63	-3.06	1.13	2.87	2.54	2.50	0.19
159	0.1 FE*NAP	0.285	1.04	0.83	-30.71	-65.49	-6.63	7.40	3.04	1.70	-2.75	0.38
160	0.1 FE*NAP	0.313	6.16	-2.78	-28.02	-76.47	-0.70	5.73	3.57	2.86	3.35	-1.02
161	0.1 CR*NAP	0.290	-2.12	3.51	1.01	-36.57	-8.72	13.30	1.95	0.05	-1.80	2.17
162	0.1 CR*NAP	0.324	3.06	1.30	-6.99	-44.90	-7.21	-3.02	1.44	0.92	2.37	1.38
163	0.1 FE*FERROCENE	0.298	-3.37	2.56	-23.20	-21.16	-24.47	-21.38	1.00	-0.46	-5.39	0.98
164	0.1 FE*FERROCENE	0.328	2.30	-0.18	9.01	-41.31	-20.89	-9.95	1.84	1.45	2.67	0.32
165	0.1 FE*FERROCENE	0.299	-4.51	1.95	11.61	-20.29	-23.54	-16.91	0.12	-0.99	-2.98	0.69
166	0.1 FE*FERROCENE	0.330	1.68	0.05	21.63	-24.17	-20.38	-11.24	1.11	-0.48	2.81	0.45
167	0.1 CO*NAP	0.298	-3.37	2.90	-9.39	-31.02	-19.43	-10.90	2.19	0.53	-4.05	1.28
168	0.1 CO*NAP	0.317	4.82	0.33	-32.18	-37.79	-11.59	-6.53	5.16	2.62	1.99	0.66

TABLE XVII (Cont'd.)

RUN	FUEL MODIFICATION	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	C BAL PCT	O BAL PCT
169	0.1 CO*NAP	0.294	-1.49	1.98	-18.04	-43.35	-16.73	-7.43	2.10	0.02	-3.27	0.92
170	0.1 CO*NAP	0.317	6.63	-0.66	-32.18	-50.23	-10.43	-6.53	4.53	2.69	3.68	0.46
171	0.1 MN*CI2	0.292	-1.38	2.37	-3.05	******	-6.95	-5.60	******	0.77	-1.71	1.39
172	0.1 MN*CI2	0.306	9.39	-1.33	-31.18	******	4.64	2.41	******	4.43	5.71	0.49
173	0.1 MN*CI2	0.301	-4.60	2.93	4.39	******	-6.79	-13.33	******	-0.41	-3.84	1.23
174	0.1 MN*CI2	0.313	6.94	-0.81	-24.38	******	0.48	-3.47	******	3.63	4.40	0.50
175	0.5 MN*CI2	0.293	-1.16	3.47	72.85	189.64	-29.23	-17.52	******	-0.24	6.74	3.02
176	0.5 MN*CI2	0.318	5.00	1.19	20.48	114.47	-22.37	-29.35	******	1.79	6.15	1.89
177	0.5 FE*FERROCENE	0.304	-5.54	5.66	88.34	58.21	-21.47	-20.59	******	-2.44	3.02	3.80
178	0.5 FE*FERROCENE	0.328	1.80	1.26	45.97	46.72	-19.77	-26.32	******	-0.60	4.49	1.44
179	0.1 MN*NAP	0.295	-2.38	3.76	37.34	******	-15.82	-13.72	-1.98	-0.71	1.60	2.6
180	0.1 MN*NAP	0.326	-13.18	7.89	33.73	******	-16.91	-12.77	-3.96	-1.65	-10.24	3.0
181	3.8 H20+N2H4.2C2H402*E	0.232	0.37	1.28	-22.01	-58.07	12.25	23.27	******	******	-2.40	0.
182	3.8 H20+N2H4.2C2H402*E	0.335	0.16	2.47	-3.17	-66.88	-2.33	-10.43	******	******	-0.04	1.
183	3.8 H20+N2H4.2C2H402*E	0.284	0.24	1.56	-9.56	156.36	-0.84	-3.51	-2.04	******	-0.88	0
184	3.8 H20+N2H4.2C2H402*E	0.290	0.15	1.88	-34.67	-27.51	0.41	7.64	0.27	0.18	-3.74	

The data obtained with unmodified [illegible] section. The experimental values for CO_2, O_2, CO, NO_x and NO_2 [illegible] cted by $(1-0.132\phi)$ and are presented on a wet basis. Table XVIII presents the unmodified Jet A data on a mole fraction basis for Can I and Table XIX presents the same data for Can II. In a similar manner Tables XX and XXI present the unmodified Jet A data in emission index units for Can I and Can II, respectively. The detailed mathematical technique for converting mole fraction measurements to emission index units is given in Appendix V.

TABLE XVIII

RUNS WITH UNMODIFIED JET A CAN I

RUN	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
1	0.353	4.19	13.3	2001	320	88	0	1597	1627	48.0	89.9	-97.0
2	0.318	3.74	13.9	2874	208	82	0	1527	1546	48.0	91.1	-96.6
3	0.318	3.88	13.9	1820	240	94	0	1595	1600	58.0	92.0	-97.1
4	0.294	3.53	13.9	2720	112	86	0	1474	1475	59.0	92.7	-94.7
5	0.312	3.64	13.4	3189	32	83	0	1523	1533	59.0	90.8	-93.6
6	0.304	3.53	14.4	3216	12	89	0	1505	1522	59.0	90.6	-97.6
7	0.340	3.62	13.9	2770	247	88	0	1543	1546	57.0	82.7	-96.9
8	0.298	3.25	14.9	6054	90	81	0	1440	1445	50.0	92.7	-99.1
9	0.312	3.48	14.5	5011	11	85	0	1500	1503	51.0	91.3	-98.6
10	0.348	4.27	0.0	2838	5	95	0	1570	1600	46.0	93.8	-100.8
11	0.308	3.50	0.0	4159	37	85	0	1535	1540	58.0	91.0	-27.9
12	0.331	3.92	0.0	2500	18	94	0	1627	1630	59.0	90.3	-30.3
13	0.294	3.56	0.0	3339	18	85	0	1523	1520	58.0	94.7	-27.5
14	0.321	4.00	0.0	1988	0	97	0	1613	1610	60.0	-93.6	-30.2
15	0.291	3.63	14.2	3452	0	83	0	1535	1542	57.0	-97.6	-96.7
16	0.286	3.59	14.1	3680	0	77	0	1500	1523	50.0	-98.8	-95.9
17	0.318	3.93	13.5	2922	0	86	0	1546	1561	46.0	-95.0	-95.6
18	0.319	4.15	13.2	1796	0	88	0	1590	1630	60.0	-97.1	-95.0
19	0.292	3.61	14.1	2573	16	86	0	1485	1536	58.0	94.7	-95.9
20	0.313	4.05	13.3	1870	30	92	0	1567	1608	60.0	96.9	-94.8
21	0.291	3.51	14.3	2453	8	83	0	14 0	1497	58.0	92.2	-96.3
22	0.325	3.97	13.5	1914	8	88	0	1567	1570	59.0	91.7	-95.8
23	0.291	3.60	14.3	3355	26	83	0	1490	1496	48.0	96.7	-97.0
24	0.316	4.12	13.1	2275	12	88	0	1580	1586	49.0	98.5	-94.4

TABLE XVIII (Cont'd.)

RUN	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
25	0.292	3.56	14.2	2581	0	88	12	1493	1500	49.0	-93.4	96.2
26	0.319	4.00	13.7	2060	0	93	15	1593	1593	50.0	-94.4	96.8
27	0.289	3.51	14.0	2155	12	87	13	1453	1470	48.0	92.1	94.7
28	0.276	3.48	14.1	2786	21	81	0	1450	1480	48.0	97.2	-94.7
29	0.320	4.02	13.2	1892	8	96	17	1550	1573	50.0	94.2	94.4
30	0.288	3.54	12.9	1371	14	86	15	1457	1457	48.0	91.2	89.3
31	0.324	4.04	12.9	1746	16	[illegible]	16	1563	1555	50.0	93.2	93.2
32	0.291	3.52	15.0	2381	15	82	15	1467	1450	47.0	92.3	99.8
33	0.327	4.12	13.9	2153	16	90	17	1607	1592	48.0	95.0	98.7
34	0.276	3.54	14.4	1880	10	81	14	1437	1473	48.0	96.4	96.3
35	0.297	3.54	14.1	2739	32	82	14	1487	1490	47.0	91.8	95.8
36	0.328	4.07	12.9	1866	22	92	17	1600	1597	48.0	93.0	93.5
37	0.293	3.51	14.3	3267	14	86	13	1497	1497	48.0	93.6	96.6
38	0.299	3.54	14.0	2377	24	83	16	1510	1504	47.0	90.4	95.3
39	0.292	3.51	14.4	3077	0	82	15	1473	1472	47.0	-93.4	97.0
40	0.324	4.02	13.4	2178	0	96	17	1588	1592	50.0	-93.6	95.6
41	0.304	3.65	14.6	4704	24	75	10	1482	1530	51.0	97.0	99.5
42	0.320	4.09	14.0	2634	16	89	13	1565	1602	54.0	97.4	98.9

TABLE XIX

RUNS WITH UNMODIFIED JET A CAN II

RUN	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
43	0.296	3.51	14.3	2354	14	77	12	1478	1482	48.0	90.5	96.5
44	0.321	4.02	13.4	1867	14	85	15	1582	1582	49.0	93.8	95.4
45	0.292	0.00	14.4	3437	0	76	12	0	0	49.0	-8.4	-80.1
46	0.316	0.00	13.7	2204	0	88	15	0	0	50.0	-4.9	-77.3
47	0.304	3.50	14.6	3840	28	73	12	1506	1516	47.0	91.4	98.6
48	0.327	4.07	13.7	2272	20	86	17	1610	1613	49.0	94.1	97.5
49	0.296	3.48	14.6	3568	20	76	19	1475	1497	49.0	92.7	98.1
50	0.315	4.17	13.5	2037	15	88	23	1608	1616	48.0	99.4	96.5
51	0.301	3.61	14.8	3745	20	75	17	1457	1492	49.0	92.3	99.5
52	0.334	4.11	13.9	2509	12	88	20	1608	1582	47.0	93.6	99.0
53	0.290	3.50	14.8	4429	22	77	19	1451	1493	50.0	97.2	99.2
54	0.300	3.53	14.6	2990	40	74	20	1472	1510	49.0	91.3	98.4
55	0.329	4.11	13.6	1937	16	87	26	1602	1630	50.0	93.7	97.2
56	0.304	3.50	14.6	3432	48	74	22	0	1463	49.0	90.5	98.5
57	0.308	3.50	14.6	3932	12	80	18	1528	1538	49.0	90.4	98.8
58	0.329	4.11	13.8	1770	8	92	23	1630	1640	51.0	93.3	98.1
59	0.310	3.48	14.8	3476	0	83	19	1538	1527	50.0	-88.3	99.6
60	0.308	3.50	14.6	4387	28	80	17	1531	1535	50.0	91.5	98.9
61	0.326	4.12	13.7	2320	0	99	27	1645	1642	51.0	-95.6	97.7
62	0.310	3.50	14.8	4411	18	81	19	1540	1528	50.0	91.0	99.9
63	0.329	4.11	13.7	2103	16	96	22	1657	1637	51.0	94.1	97.7
64	0.309	3.50	14.6	3740	14	78	21	1510	1483	51.0	89.7	98.8
65	0.328	4.12	13.6	2608	12	95	26	1610	1580	52.0	95.7	97.4
66	0.297	3.48	14.8	4589	18	76	22	1535	1515	48.0	96.4	99.2

TABLE XIX (Cont'd.)

RUN	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
67	0.327	4.12	13.8	2799	16	94	34	1627	1622	47.0	96.4	98.3
68	0.301	3.50	14.8	3984	10	78	19	1543	1533	49.0	92.6	99.5
69	0.292	3.56	14.8	5766	50	81	19	1513	1478	50.0	101.3	99.9
70	0.304	4.13	14.0	4032	8	92	25	1613	1542	48.0	106.6	98.8
71	0.304	3.50	14.8	4848	10	76	23	1503	1507	50.0	93.7	99.8
72	0.332	4.06	13.7	2103	14	92	34	1655	1640	47.0	92.2	97.6
73	0.312	3.50	13.8	5131	18	75	19	0	0	49.5	92.1	95.7
74	0.332	4.16	13.2	3107	20	92	30	0	0	50.5	96.5	95.9
75	0.321	4.12	14.0	3473	14	85	26	1578	1615	50.0	99.6	99.4
76	0.307	3.50	14.8	4656	14	77	19	1518	1547	48.0	92.4	100.0
77	0.329	4.14	13.9	2656	16	87	27	1610	1638	49.0	95.9	99.1
78	0.319	3.52	14.9	4790	12	77	20	1510	1525	48.5	89.7	101.3
79	0.284	4.10	14.0	2565	12	87	25	1590	1626	52.0	109.6	97.8
80	0.291	3.49	14.9	5026	16	78	19	1513	1527	49.0	98.1	99.8
81	0.314	4.07	14.0	3329	10	87	23	1565	1593	49.5	100.3	98.9
82	0.301	3.48	14.9	5040	32	77	19	0	1495	48.5	94.7	100.1
83	0.322	4.04	14.0	3445	12	85	23	0	1588	49.0	97.5	99.2
84	0.294	3.48	14.9	5286	14	76	19	0	1511	48.5	97.5	100.4
85	0.322	4.14	14.1	2680	8	83	25	0	1623	49.5	98.0	99.8
86	0.293	3.48	15.0	4300	18	79	19	1502	1482	49.5	95.4	100.3
87	0.323	4.07	14.1	2440	6	92	26	1620	1608	50.5	95.6	99.4
88	0.291	3.51	15.1	4281	0	81	19	1487	1495	48.5	-96.7	100.9
89	0.313	4.08	14.2	2350	0	92	25	0	1600	49.0	-98.6	99.9
90	0.292	3.48	15.1	4565	0	80	19	1450	1497	49.0	-96.3	100.8

TABLE XIX (Cont'd.)

RUN	PHI	CO2 PCT	O2 PCT	CO PPM	HC PPM	NOX PPM	NO2 PPM	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
91	0.314	4.10	14.2	2587	0	87	23	1610	1558	49.0	-99.3	99.8
92	0.290	3.54	14.9	3391	18	86	19	1513	0	47.5	95.6	99.6
93	0.322	4.07	13.7	2273	12	100	23	1670	0	48.5	95.6	97.4

TABLE XX

RUNS WITH UNMODIFIED JET A CAM I

RUN	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
1	0.353	2710.	6258.	82.3	7.52	5.95	0.00	1597	1627	48.0	89.9	-97.0
2	0.319	2679.	7243.	131.0	5.41	6.14	0.00	1527	1546	48.0	91.1	-96.6
3	0.318	2780.	7243.	82.9	6.25	7.04	0.00	1596	1600	58.0	92.0	-97.1
4	0.294	2731.	7822.	133.9	3.15	6.95	0.00	1474	1475	59.0	92.7	-94.7
5	0.312	2657.	7114.	148.1	0.84	6.33	0.00	1523	1533	59.0	90.8	-93.6
6	0.304	2643.	7842.	153.2	0.32	6.96	0.00	1505	1522	59.0	90.6	-97.6
7	0.340	2429.	6784.	118.3	6.02	6.17	0.00	1543	1546	57.0	92.7	-96.9
8	0.298	2481.	8275.	294.1	2.49	6.46	0.00	1440	1445	50.0	92.7	-99.1
9	0.312	2540.	7698.	232.7	0.29	6.48	0.00	1500	1503	51.0	91.3	-98.6
10	0.348	2801.	6680.	118.4	0.11	6.51	0.00	1570	1600	46.0	93.8	-100.8
11	0.308	2587.	0.	195.6	0.99	6.56	0.00	1533	1540	58.0	91.0	-27.9
12	0.331	2700.	0.	109.6	0.45	6.77	0.00	1627	1630	59.0	90.3	-30.3
13	0.294	2754.	0.	164.4	0.50	6.87	0.00	1523	1520	58.0	94.7	-27.5
14	0.321	2840.	0.	89.8	0.00	7.20	0.00	1613	1610	60.0	-93.6	-30.2
15	0.291	2837.	8072.	171.7	0.00	6.78	0.00	1525	1542	57.0	-97.6	-96.7
16	0.286	2854.	8152.	186.1	0.00	6.40	0.00	1500	1523	50.0	-98.8	-95.9
17	0.318	2816.	7035.	133.2	0.00	6.44	0.00	1546	1561	46.0	-95.0	-95.6
18	0.319	2964.	6857.	81.6	0.00	6.57	0.00	1590	1630	60.0	-97.1	-95.0
19	0.292	2812.	7988.	127.5	0.45	7.00	0.00	1485	1536	58.0	94.7	-95.9
20	0.313	2947.	7039.	86.6	0.79	6.99	0.00	1567	1608	60.0	96.9	-94.8
21	0.291	2743.	8129.	122.0	0.22	6.78	0.00	1430	1497	58.0	92.2	-96.3
22	0.325	2784.	6886.	85.4	0.20	6.45	0.00	1567	1570	59.0	91.7	-95.8
23	0.291	2813.	8129.	166.8	0.73	6.78	0.00	1490	1496	48.0	96.7	-97.0
24	0.316	2970.	6869.	104.3	0.31	6.63	0.00	1580	1586	49.0	98.5	-94.4

TABLE XX (Cont'd.)

RUN	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
25	0.292	2773.	8045.	127.9	0.00	7.16	0.97	1493	1500	49.0	-93.4	96.2
26	0.319	2857.	7117.	93.6	0.00	6.94	1.12	1593	1593	50.0	-94.4	96.8
27	0.289	2762.	8012.	107.9	0.34	7.15	1.06	1453	1470	48.0	92.1	94.7
28	0.276	2865.	8442.	145.9	0.02	6.97	0.00	1450	1480	53.0	97.2	-94.7
29	0.320	2862.	6836.	85.7	0.20	7.14	1.26	1550	1573	50.0	94.2	94.4
30	0.288	2795.	7408.	68.8	0.40	7.09	1.23	1457	1457	48.0	91.2	89.3
31	0.324	2842.	6600.	78.1	0.40	6.98	1.17	1563	1555	50.0	93.2	93.2
32	0.291	2751.	8527.	118.4	0.42	6.70	1.22	1467	1450	47.0	92.3	99.8
33	0.327	2872.	7048.	95.5	0.40	6.56	1.23	1607	1592	48.0	95.0	98.7
34	0.276	2914.	8622.	98.4	0.29	6.97	1.20	1437	1473	48.0	96.4	96.3
35	0.297	2712.	7856.	133.5	0.89	6.56	1.12	1487	1490	47.0	91.8	95.8
36	0.328	2829.	6521.	82.5	0.55	6.68	1.23	1600	1597	48.0	93.0	93.5
37	0.293	2725.	8074.	161.4	0.39	6.98	1.21	1497	1497	48.0	93.6	96.6
38	0.299	2694.	7749.	115.1	0.66	6.60	1.27	1510	1504	47.0	90.4	95.3
39	0.292	2734.	8158.	152.5	0.00	6.67	1.22	1473	1472	47.0	-93.4	97.0
40	0.324	2828.	6856.	97.5	0.00	7.06	1.25	1588	1592	50.0	-93.6	95.6
41	0.304	2733.	7951.	224.1	0.65	5.87	0.78	1482	1530	51.0	97.0	99.5
42	0.320	2912.	7251.	119.3	0.41	6.62	0.96	1565	1602	54.0	97.4	98.9

TABLE XXI

RUNS WITH UNMODIFIED JET A CAN II

RUN	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	C BAL PCT
43	0.296	2698.	7994.	115.1	0.39	6.18	0.96	1478	1482	48.0	90.5	96.5
44	0.321	2854.	6919.	84.3	0.36	6.30	1.11	1582	1582	49.0	93.8	95.4
45	0.292	0.	8158.	170.3	0.00	6.18	0.97	0	0	49.0	-8.4	-80.1
46	0.316	0.	7183.	101.1	0.00	6.63	1.13	0	0	50.0	-4.9	-77.3
47	0.304	2621.	7951.	182.9	0.62	5.71	0.93	1506	1516	47.0	91.4	98.6
48	0.327	2837.	6947.	100.8	0.50	6.26	1.23	1610	1613	49.0	94.1	97.5
49	0.296	2675.	8162.	174.5	0.55	6.10	1.52	1475	1497	49.0	92.7	98.1
50	0.315	3015.	7100.	93.7	0.39	6.65	1.73	1608	1616	48.0	99.4	96.5
51	0.301	2654.	8139.	180.2	0.54	5.92	1.34	1457	1492	49.0	92.3	99.5
52	0.334	2806.	6904.	109.0	0.29	6.28	1.42	1608	1582	47.0	93.6	99.0
53	0.290	2745.	8441.	221.0	0.62	6.31	1.55	1451	1493	50.0	97.2	99.2
54	0.300	2678.	8055.	144.3	1.10	5.86	1.58	1472	1510	49.0	91.3	98.4
55	0.329	2848.	6855.	85.4	0.40	6.30	1.88	1602	1630	50.0	93.7	97.2
56	0.304	2621.	7951.	163.5	1.30	5.79	1.72	0	1463	49.0	90.5	98.5
57	0.308	2587.	7850.	184.9	0.32	6.18	1.39	1528	1538	49.0	90.4	98.8
58	0.329	2848.	6956.	78.0	0.20	6.66	1.66	1630	1640	51.0	93.3	98.1
59	0.310	2556.	7907.	162.5	0.00	6.37	1.45	1538	1527	50.0	-88.3	99.6
60	0.308	2587.	7850.	206.4	0.75	6.18	1.31	1531	1535	50.0	91.5	98.9
61	0.326	2881.	6967.	103.2	0.00	7.23	1.97	1645	1642	51.0	-95.6	97.7
62	0.310	2571.	7907.	206.2	0.48	6.22	1.45	1540	1528	50.0	91.0	99.9
63	0.329	2848.	6905.	92.7	0.40	6.95	1.59	1657	1637	51.0	94.1	97.7
64	0.309	2579.	7825.	175.4	0.37	6.00	1.61	1510	1483	51.0	89.7	98.8
65	0.328	2864.	6975.	115.3	0.30	6.90	1.88	1610	1580	52.0	95.7	97.4
66	0.292	2710.	8385.	227.4	0.50	6.18	1.79	1535	1515	48.0	96.4	99.2

TABLE XXI (Cont'd.)

RUN	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
67	0.327	2872.	6997.	124.1	0.40	6.85	2.47	1627	1622	47.0	96.4	98.3
68	0.301	2646.	8139.	191.7	0.27	6.16	1.50	1543	1533	49.0	92.6	99.5
69	0.292	2773.	8385.	285.8	1.41	6.59	1.54	1513	1478	50.0	101.3	99.9
70	0.304	3092.	7624.	192.1	0.21	7.20	1.95	1613	1542	48.0	106.6	98.8
71	0.304	2621.	8060.	231.0	0.27	5.95	1.80	1503	1507	50.0	93.7	99.8
72	0.332	2789.	6844.	91.9	0.34	6.60	2.44	1655	1640	47.0	92.2	97.6
73	0.312	2555.	7364.	238.3	0.47	5.72	1.45	0	0	49.5	92.1	95.7
74	0.332	2857.	6599.	135.8	0.49	6.60	2.15	0	0	50.5	96.5	95.9
75	0.321	2925.	7247.	156.9	0.36	6.30	1.92	1578	1615	50.0	99.6	99.4
76	0.307	2595.	7999.	219.7	0.37	5.97	1.47	1518	1547	48.0	92.4	100.0
77	0.329	2869.	7016.	117.1	0.40	6.30	1.95	1610	1638	49.0	95.9	99.1
78	0.319	2514.	7782.	217.7	0.31	5.75	1.49	1510	1525	48.5	89.7	101.3
79	0.284	3282.	8180.	130.6	0.34	7.28	2.09	1590	1626	52.0	109.6	97.8
80	0.291	2727.	8475.	249.9	0.45	6.37	1.55	1513	1527	49.0	98.1	99.0
81	0.314	2952.	7407.	153.6	0.26	6.59	1.74	1565	1593	49.5	100.3	98.9
82	0.301	2631.	8194.	242.5	0.87	6.08	1.50	0	1495	48.5	94.7	100.1
83	0.322	2859.	7243.	155.1	0.30	6.29	1.70	0	1588	49.0	97.5	99.2
84	0.294	2692.	8436.	260.3	0.39	6.14	1.53	0	1511	48.5	97.5	100.4
85	0.322	2930.	7268.	120.7	0.20	6.51	1.85	0	1623	49.5	98.0	99.8
86	0.293	2701.	8492.	212.4	0.50	6.41	1.54	1502	1482	49.5	95.4	100.3
87	0.323	2872.	7246.	109.5	0.15	6.78	1.91	1620	1608	50.5	95.6	99.4
88	0.291	2743.	8612.	212.9	0.00	6.61	1.55	1487	1495	48.5	-96.7	100.9
89	0.313	2969.	7563.	108.8	0.00	6.99	1.90	0	1600	49.0	-98.6	99.9
90	0.292	2710.	8577.	226.3	0.00	6.51	1.54	1450	1497	49.0	-96.3	100.8

TABLE XXI (Cont'd.)

RUN	PHI	EICO2 POUNDS	EIO2 PER	EICO 1000	EIHC POUNDS	EINOX OF	EINO2 FUEL	TE F	TP F	P PSIG	C BAL PCT	O BAL PCT
91	0.314	2974.	7508.	119.4	0.00	6.59	1.74	1610	1558	49.0	-99.3	99.8
92	0.290	2776.	8504.	169.2	0.51	7.05	1.55	1513	0	47.5	95.6	99.6
93	0.327	2880.	7068.	102.3	0.30	7.40	1.70	1670	0	48.5	95.6	97.4

// XEQ L80

APPENDIX V

MATERIAL BALANCE CALCULATIONS

The general chemical equation for burning in excess air can be approximated by,

$$CH_n + \frac{1}{\phi}\left(1 + \frac{n}{4}\right)\left[O_2 + 3.76\ N_2\right] = CO_2 + \frac{n}{2}H_2O + \frac{1}{\phi}\left(1 + \frac{n}{4}\right) 3.76\ N_2 + \left(\frac{1}{\phi} - 1\right)\left(1 + \frac{n}{4}\right) O_2 \qquad (10)$$

Assumed in equation (10) is that the CO and CO_2 levels in the reactant air are negligible and that the CO and unburned hydrocarbon levels in the product stream can be neglected as a first approximation. These assumptions have been confirmed experimentally.

The stoichiometric air to fuel ratio $(A/F)_s$, can be calculated as a function of hydrogen to carbon ratio, n.

$$(A/F)_s = \frac{4.76\ (1 + n/4)}{1} \qquad \left(\frac{29}{12 + n}\right) = 34.51\left(\frac{4 + n}{12 + n}\right) \qquad (11)$$

Similarly, equivalence ratio can be expressed as a function of n and operating air to fuel ratio $(A/F)_o$.

$$\phi \equiv (A/F)_s\ (F/A)_o = 34.51\left(\frac{4 + n}{12 + n}\right)\ (F/A)_o \qquad (12)$$

In order to calculate the expected volume percent of CO_2, H_2O, and O_2 in the combustion effluent stream, the mole ratio of reactant air to product gases, B, must be obtained.

$$B = \frac{1/\phi\ (1 + n/4)\ 4.76}{1 + \frac{n}{2} + \frac{1}{\phi}\ (1 + \frac{n}{4})\ 3.76 + (\frac{1}{\phi} - 1)\ (1 + \frac{n}{4})} \qquad (13)$$

which reduces to:

$$B = \frac{4.76\ (4 + n)}{n\phi + 4.76\ (4 + n)} \tag{14}$$

The volume percent carbon in the effluent stream can be calculated assuming that unburned hydrocarbons are expressed as methane.

$$\% C = \% (CO_2 + CO + CH_4) = (F/A)_o \left(\frac{29}{12 + n}\right) B\ 100 \tag{15}$$

Substituting equation (12) into (15) the equation for carbon volume percent as a function of n and ϕ is obtained.

$$\% C = \frac{400\ \phi}{n\phi + 4.76\ (4 + n)} \tag{16}$$

The volume percent water is simply the volume percent carbon multiplied by n/2.

$$\% H_2O = \frac{200\ n\phi}{n\phi + 4.76\ (4 + n)} \tag{17}$$

The volume percent oxygen can be calculated by multiplying the volume percent carbon by $(1/\phi - 1)\ (1 + n/4)$.

$$\% O_2 = \frac{100\ (1 - \phi)\ (4 + n)}{n\phi + 4.76\ (4 + n)} \tag{18}$$

Using the experimentally determined hydrogen to carbon ratio of 1.89 for Jet A fuel, then the predicted emission mole fractions in the range of $.27 < \phi < .34$ are:

$$\% (CO_2 + CO + CH_4) = 13.8\ \phi \tag{19}$$

$$\% O_2 = 20.6\ (1 - \phi) \tag{20}$$

$$\% H_2O = 13.2\phi \tag{21}$$

$$B = .977 \tag{22}$$

The correction factor for reporting CO, CO_2, NO_x, and O_2 on a wet basis is therefore:

$$(1 - 0.132\ \phi). \tag{23}$$

Additional corrections for CO_2 and CO present in the air originally can be added to the material balance equations listed above if additional accuracy is desired. This correction was found unnecessary for the results reported here.

The material balance equations used to compute the carbon balance and oxygen balance reported in Appendices I and IV are:

$$\% C = \frac{\text{measured mole fraction of carbon components}}{\text{Equation 16}} \times 100 \qquad (24)$$

$$\% C = \frac{(\% CO_2 + 10^{-4} \text{ ppm CO} + 10^{-4} \text{ ppm HC})(n\phi + 4.76(4+n))}{4\phi} \qquad (25)$$

$$\% O_2 = \frac{\text{measured mole fraction of oxygen components} + 1/2(\text{Equation 8})}{\text{Equation 16} + 1/2(\text{Equation 17}) + \text{Equation 18}} \qquad (26)$$

$$\% O_2 = \frac{(\% CO_2 + \% O_2 + 5 \times 10^{-5} \text{ ppm CO} + 5 \times 10^{-5} \text{ ppm } (NO_x - NO_2) + 10^{-4} \text{ ppm } NO_2) + 100\, n\phi/(n\phi + 4.76\ (4+n))}{(4+n)/(n\phi + 4.76\ (4+n))} \qquad (27)$$

Equations (25) and (27) reduce to:

$$\% C = \frac{(1.89\phi + 28.04)}{4\phi} \text{ (measured mole fraction of carbon components)} \qquad (28)$$

$$\% O_2 = 32.1\phi + (0.321\phi + 4.76)\text{(measured mole fraction of oxygen compounds)} \qquad (29)$$

In order to convert the mole fraction of a component i in the combustion effluent stream to emission index in lb per 1000 lb of fuel, one multiplies the mole fraction value by the molecular weight of i and by equation (11) and divides the product by equations (12), (14) and the molecular weight of air. The resulting expression is:

$$EI_i = X_i \left(\frac{A}{F}\right)_s \frac{(n\phi + 4.76\ (4+n))}{4.76\ (4+n)} \frac{(MW)_i}{29} \frac{10^3}{\phi} \qquad (30)$$

The symbols are defined on page 36.

Since n = 1.89 and $(A/F)_s$ = 14.6 for Jet A, Equation (30) reduces to:

$$EI_i = X_i \, (MW)_i \, (33.9 + \frac{503}{\phi}) \qquad (31)$$

Equation (31) was used to compute the emission index values for Tables XV, XX and XXI. Similarly, one can calculate the emission index of any effluent species if the hydrogen to carbon ratio of the fuel and the equivalence ratios are known.

APPENDIX VI

KINETICS OF NO FORMATION IN GAS TURBINE COMBUSTORS

The mechanism for NO formation in hot air was described in the Introduction and is summarized below:

$$M + O_2 \underset{2}{\overset{1}{\rightleftharpoons}} 2O + M \tag{1}$$

$$O + N_2 \underset{4}{\overset{3}{\rightleftharpoons}} NO + N \tag{2}$$

$$N + O_2 \underset{6}{\overset{5}{\rightleftharpoons}} NO + O \tag{3}$$

$$N + OH \underset{8}{\overset{7}{\rightleftharpoons}} NO + H \tag{4}$$

where reactions 2 and 3 are referred to as the Zeldovich chain mechanism.

In Table XXII are listed the mole fractions of all combustion product species with a mole fraction greater than 5×10^{-8} based on equilibrium calculations (5). The calculations were run assuming 4 atmosphere pressure and an air preheat of 400°F (478°K) using a fuel with a carbon to hydrogen ratio of 1.9185. This is representative of the Esso High Pressure Cannular Combustor using Jet A fuel. The mole fraction of nitrogen atoms, at equilibrium, never achieves a significant level. One can, therefore, make the steady state assumption for nitrogen atoms, $(N) = 0$. The steady state value for nitrogen atoms is:

$$(N)_{ss} = (O)\left[\frac{k_3(N_2) + k_6(NO) + k_8(H)(NO)(O)^{-1}}{k_4(NO) + k_5(O_2) + k_7(OH)}\right] \tag{32}$$

where the brackets are used to indicate concentration in moles cm^{-3}.

The rate of production of nitric oxide is:

$$(NO) = k_3(O)(N_2) - k_4(N)(NO) + k_5(O_2)(N) - k_6(NO)(O) + k_7(OH)(N) - k_8(H)(NO) \tag{33}$$

TABLE XXII

EQUILIBRIUM CALCULATION
JET A ($C_1H_{1.9185}$) at 58.8 PSIA
AIR PREHEAT = 478°K (400°F)

ϕ	0.30	0.35	0.40	0.60	0.80	0.90	0.95	1.00	1.10	1.30	1.50
Ar	9.15-3	9.12-3	9.09-3	8.97-3	8.84-3	8.76-3	8.71-3	8.65-3	8.49-3	8.09-3	7.72-3
CO			1.17-7	3.69-5	1.27-3	4.83-3	8.66-3	1.47-2	3.53-2	8.46-2	1.23-1
CO_2	4.31-2	5.00-2	5.68-2	8.35-2	1.08-1	1.17-1	1.19-1	1.19-1	1.09-1	7.78-2	5.60-2
H				6.24-7	3.45-5	1.39-4	2.43-4	3.81-4	6.33-4	5.76-4	3.23-4
HCO								5.74-8	2.28-7	7.62-7	1.07-5
HNO					6.39-8	1.19-7	1.39-7	1.42-7	8.99-8		
HO_2				3.74-7	1.08-6	1.10-6	9.22-7	6.40-7	1.57-7		
H_2				8.84-6	2.34-4	8.36-4	1.50-3	2.61-3	7.15-3	2.58-2	5.27-2
H_2O	3.85-2	4.51-2	5.16-2	7.72-2	1.01-1	1.12-1	1.17-1	1.21-1	1.27-1	1.27-1	1.16-1
H_2O_2					1.24-7	1.43-7	1.34-7	1.09-7			
NO	1.83-4	3.78-4	6.75-4	2.85-3	5.01-3	4.83-3	4.19-3	3.23-3	1.23-3	1.10-4	1.18-5
NO_2	4.89-6	5.93-6	6.80-6	7.97-6	5.29-6	3.02-6	1.92-6	1.02-6	1.50-7		
N_2	7.64-1	7.61-1	7.58-1	7.47-1	7.35-1	7.29-1	7.25-1	7.21-1	7.08-1	6.76-1	6.45-1
N_2O			7.32-8	2.85-7	4.86-7	4.65-7	4.02-7	3.09-7	1.17-7		
O			2.34-7	2.06-5	2.05-4	3.43-4	3.62-4	3.17-4	1.22-4	6.55-6	3.65-7
OH	1.26-6	5.93-6	1.71-5	3.77-4	1.97-3	3.01-3	3.29-3	3.22-3	2.05-3	4.23-4	8.26-5
ϕ	0.30	0.35	0.40	0.60	0.80	0.90	9.95	1.00	1.10	1.30	1.50
O_2	1.45-1	1.34-1	1.24-1	8.00-2	3.78-2	1.94-2	1.19-2	6.20-3	9.16-4	1.37-5	3.46-7
NH_3										1.93-7	6.90-7
HCN											7.03-8
HO_2				3.24-7	1.08-6						
T°K	1205	1316	1424	1820	2162	2300	2352	2388	2389	2245	2085
t°F	1709	1909	2103	2816	3432	3680	3774	3838	3840	3581	3293
A/F	50.8	43.3	37.6	24.8	18.5	16.4	15.5	14.7	13.4	11.3	9.77
$10^3T^{-1}°K^{-1}$	0.830	.760	0.702	0.549	0.463	0.435	0.425	0.419	0.419	0.445	0.480
δ			0.148	0.450	0.752	0.774	0.773	0.661	0.460		
θ			1.34-5	0.0701	8.78	39.8	69.1	98.3	98.4		

The addition of $\dot{(N)} + \dot{(NO)}$ gives the following equation:

$$\frac{d(NO)}{dt} = \dot{(NO)} = 2k_3(O)\left[N_2 - \frac{k_4(NO)(N)}{k_3(O)}\right] \qquad (34)$$

Substituting equation (32) into (34) and making use of the equilibrium relationships,

$$K_{NO} = \frac{k_3}{k_4}\frac{k_5}{k_6} = \frac{(NO)_e^2}{(O_2)_e(N_2)_e} \quad \text{and} \quad \frac{k_3}{k_4}\frac{k_7}{k_8} = \frac{(NO)_e^2\,(H)_e}{(O)_e(OH)_e(N_2)_e}$$

the following equation is obtained.

$$\dot{(NO)} = 2k_3(O)(N_2)_e \left[\frac{k_5(O_2)_e\left[\frac{(O_2)}{(O_2)_e}\frac{(N_2)}{(N_2)_e} - \left(\frac{(NO)}{(NO)_e}\right)^2\right] + k_7(OH)_e\left[\frac{(N_2)}{(N_2)_e}\frac{(OH)}{(OH)_e} - \left(\frac{(NO)}{(NO)_e}\right)^2\frac{(O)_e\,(H)}{(O)\,(H)_e}\right]}{k_4(NO) + k_5(O_2) + k_7(OH)}\right] \qquad (35)$$

Since the equilibrium mole fraction of NO is always small compared to the major combustion products ($CO_2 + H_2O$) one can assume that the NO producing reactions add little heat to the flame. The combustion reactions can, therefore, be assumed to take place at the adiabatic flame temperature and the primary combustion species are assumed at equilibrium. Equation (35) can now be simplified to:

$$\frac{d\rho}{dt} = \dot{\rho} = \frac{2k_3(O)_e(N_2)_e}{(NO)_e}\left[1 - \rho^2\right]\left[\frac{1}{1 + \frac{k_4\,\rho}{k_5\frac{(O_2)_e}{(NO)_e} + k_7\frac{(OH)_e}{(NO)_e}}}\right] \tag{36}$$

where $\rho = \frac{(NO)}{(NO)_e}$.

Making use of the equilibrium constants $K_o = (O)_e^2/(O_2)_e$ and K_{NO} which was previously defined, the desired solution for $\dot{\rho}$ is obtained.

$$\dot{\rho} = \frac{2k_3K_o^{1/2}(N_2)_e^{1/2}}{K_{NO}^{1/2}(RT)^{1/2}}\left[\frac{1 - \rho^2}{1 + \frac{k_4K_{NO}^{1/2}(N_2)_e^{1/2}}{k_5(O_2)_e^{1/2}}\left(1 + \frac{k_7(OH)_e}{k_5(O_2)_e}\right)\rho}\right] \tag{37}$$

Equation (37) is integrated to give

$$(\delta + 1)\ln(1-\rho) + (\delta-1)\ln(1 + \rho) = -\theta t \tag{5}$$

where,

$$\delta = \frac{\frac{k_4}{k_5}K_{NO}^{\frac{1}{2}}\left(\frac{X_{N_2}}{X_{O_2}}\right)^{\frac{1}{2}}}{1 + \frac{k_7}{k_5}\left(\frac{X_{OH}}{X_{O_2}}\right)} \tag{38}$$

X_i = mole fraction of component i.

P = pressure in atmospheres.

R = gas constant = 82.057 $\frac{cm^3\ atm}{mole\ °K}$ = 1.987 $\frac{cal}{mole\ °K}$.

T = temperature in °K

$$\theta = \frac{4k_3K_o^{1/2}P^{1/2}X_{N_2}^{1/2}}{K_{NO}^{1/2}RT} \tag{39}$$

The following values for the rate constants (32) and a calculated value for k_7 based on collisio .. ory were used to evaluate δ and Θ.

$$k_3 = 1.36 \times 10^{14} \exp\left[-75{,}400/RT\right] \quad cm^3\ mole^{-1}\ sec^{-1}$$

$$k_4 = 3.10 \times 10^{13} \exp\left[-334/RT\right] \quad cm^3\ mole^{-1}\ sec^{-1}$$

$$k_5 = 6.43 \times 10^{9}\ T \exp\left[-6250/RT\right] \quad cm^3\ mole^{-1}\ sec^{-1}$$

$$k_7 = 7.25 \times 10^{11}\ T^{\frac{1}{2}} \quad cm^3\ mole^{-1}\ sec^{-1}$$

The value for k_7 was based on a collision diameter of 4.7Å for OH and 2.7A for N. The equilibrium constants $k_o^{1/2}$ and $K_{NO}^{1/2}$ were determined by at least squares fit of the JANAF values (33) over the temperature range 1000°K to 2500°K.

$$K_o^{1/2} = 2.90 \times 10^{3} \exp\left[-60{,}755/RT\right]\ atm^{1/2}$$

$$K_{NO}^{1/2} = 4.52 \exp\left[-21{,}583/RT\right]$$

The numerical expressions for δ and Θ are:

$$\rho = \frac{2.18 \times 10^{4}\ T^{-1} \exp\left(-15{,}665/RT\right) \left(\frac{X_{N_2}}{X_{O_2}}\right)^{\frac{1}{2}}}{1 + 1.13 \times 10^{2}\ T^{-\frac{1}{2}} \exp\left(6250/RT\right)\left(\frac{X_{OH}}{X_{O_2}}\right)} \qquad (40)$$

$$\theta = 4.24 \times 10^{15}\ T^{-1}\ P^{\frac{1}{2}}\ X_{N_2}^{\frac{1}{2}} \left(\exp - 114{,}572/RT\right)\ sec^{-1} \qquad (41)$$

The value for δ and Θ for the equivalence ratios 0.8 to 1.1 are included in Table XXII. The time required, in milliseconds, to achieve a particular fraction of the NO equilibrium value is tabulated in Table XXIII.

TABLE XXIII

TIME TO ACHIEVE A PARTICULAR ρ

	Equivalence Ratio				
ρ	0.8	0.9	0.95	1.0	1.1
0.01	1.72	0.391	0.225	0.136	0.0095
0.05	8.86	2.01	1.16	0.698	0.493
0.1	18.3	4.16	2.39	1.45	1.04
0.2	39.4	8.91	5.13	3.14	2.31
0.3	63.8	14.4	8.29	5.11	3.85
0.4	92.4	20.9	12.0	7.47	5.73
0.5	127	28.6	16.5	10.3	8.06

Equation (5) can be simplified for the conditions generally applicable to gas turbine combustors by substituting a series approximation for the natural logarithms.

$$\ln (1 - \rho) = -\rho - 1/2\rho^2 - 1/3\rho^3 - 1/4\rho^4 - \ldots\ldots \quad (42)$$

$$\ln (1 - \rho) = \rho - 1/2\rho^2 + 1/3\rho^3 + 1/4\rho^4 - \ldots\ldots \quad (43)$$

The following expression is obtained.

$$\rho\left(2 + \frac{2}{3}\rho^2 + \rho\delta + \frac{\rho^3\delta)}{2}\right) = \theta t \quad (44)$$

which can be simplified for $\rho<0.2$ and $\delta<0.8$ to:

$$\rho = \frac{\theta t}{2} \quad (6)$$

The errors involved in using the approximate equation (6) are listed in Table XXIV.

TABLE XXIV

RANGE OF ERRORS IN USING EQUATION (6)

ρ	δ	θt Exact Equation(1)	θt Approximate Equation(5)	Error %
0.1	0.8	0.209	0.2	4.3
0.2	0.8	0.438	0.4	8.7
0.3	0.8	0.694	0.6	13.5
0.4	0.8	0.987	0.8	18.9
0.3	1.2	0.732	0.6	18.0
0.3	1.0	0.713	0.6	15.8
0.3	0.6	0.675	0.6	11.1
0.3	0.4	0.657	0.6	8.7
0.3	0.2	0.638	0.6	6.0
0.3	0	0.619	0.6	3.1

Figure 15 shows the effect of temperature on ρ as a function of equivalence ratio. Equation (6) overpredicts the NO mole fraction by less than 9% in the range of interest.

The empirical rate constant Θ behaves like a true rate constant over the range of interest for NO_x kinetics in combustion. The mole fraction of nitrogen is essentially constant and the pressure is usually constant in a combustor.

A tabulation of equilibrium mole fraction of NO_x as a function of temperature and equivalence ratio is included in Table XXV. Not that Θ is essentially independent of equivalence ratio. An Arrhenius plot of Θ is given in Figure 16. Using Table XXV and Figure 16, it is possible to calculate the Zeldovich NO_x mole fraction in one step. For example, assuming that combustion of fuel droplets occurs on the droplet surface at an equivalence ratio of one, at the adiabatic flame temperature, and the residence time in the primary zone is proportional to the fuel rate, then the data in Table XXVI are obtained.

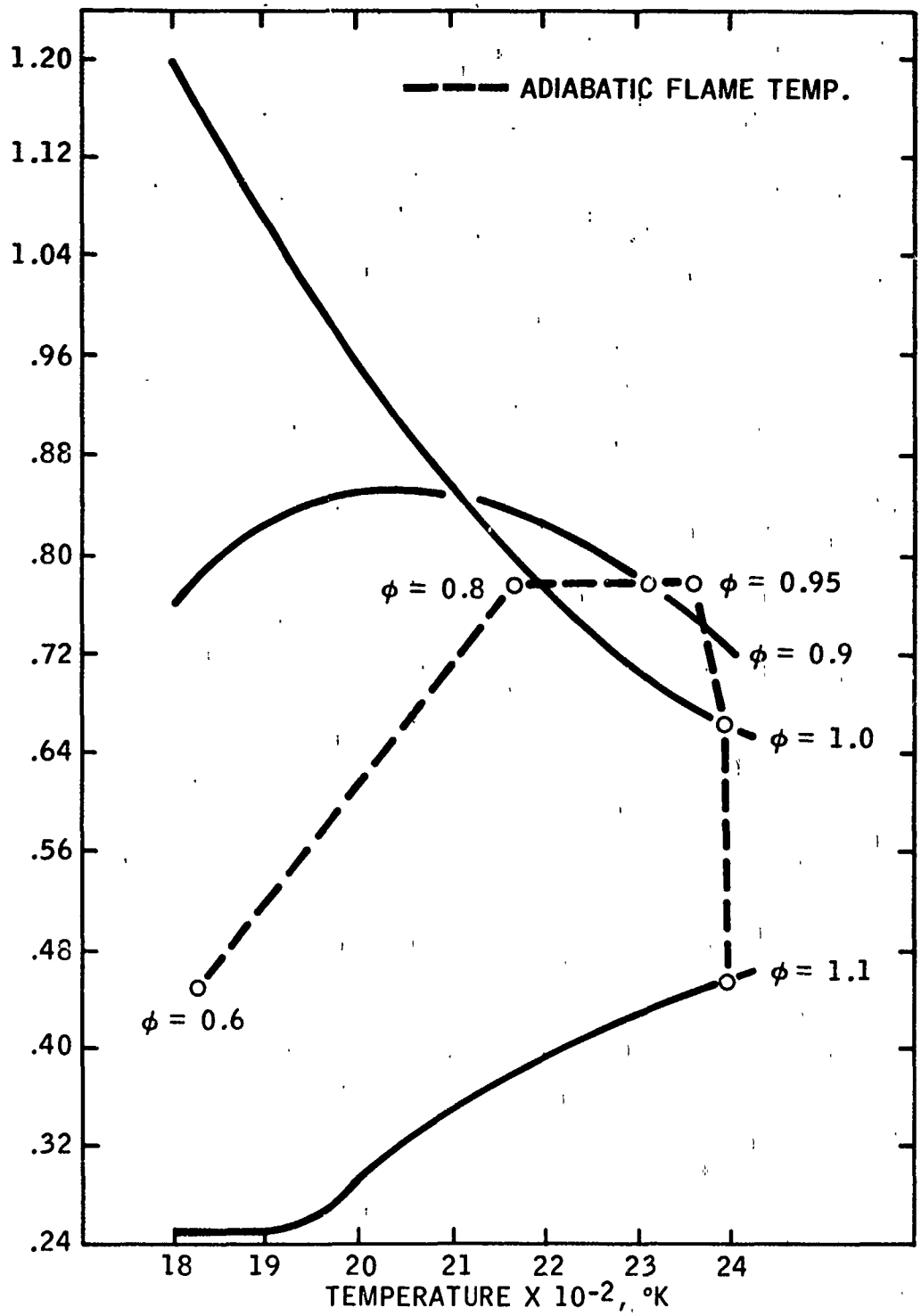

Figure 15

EFFECT OF TEMPERATURE ON S

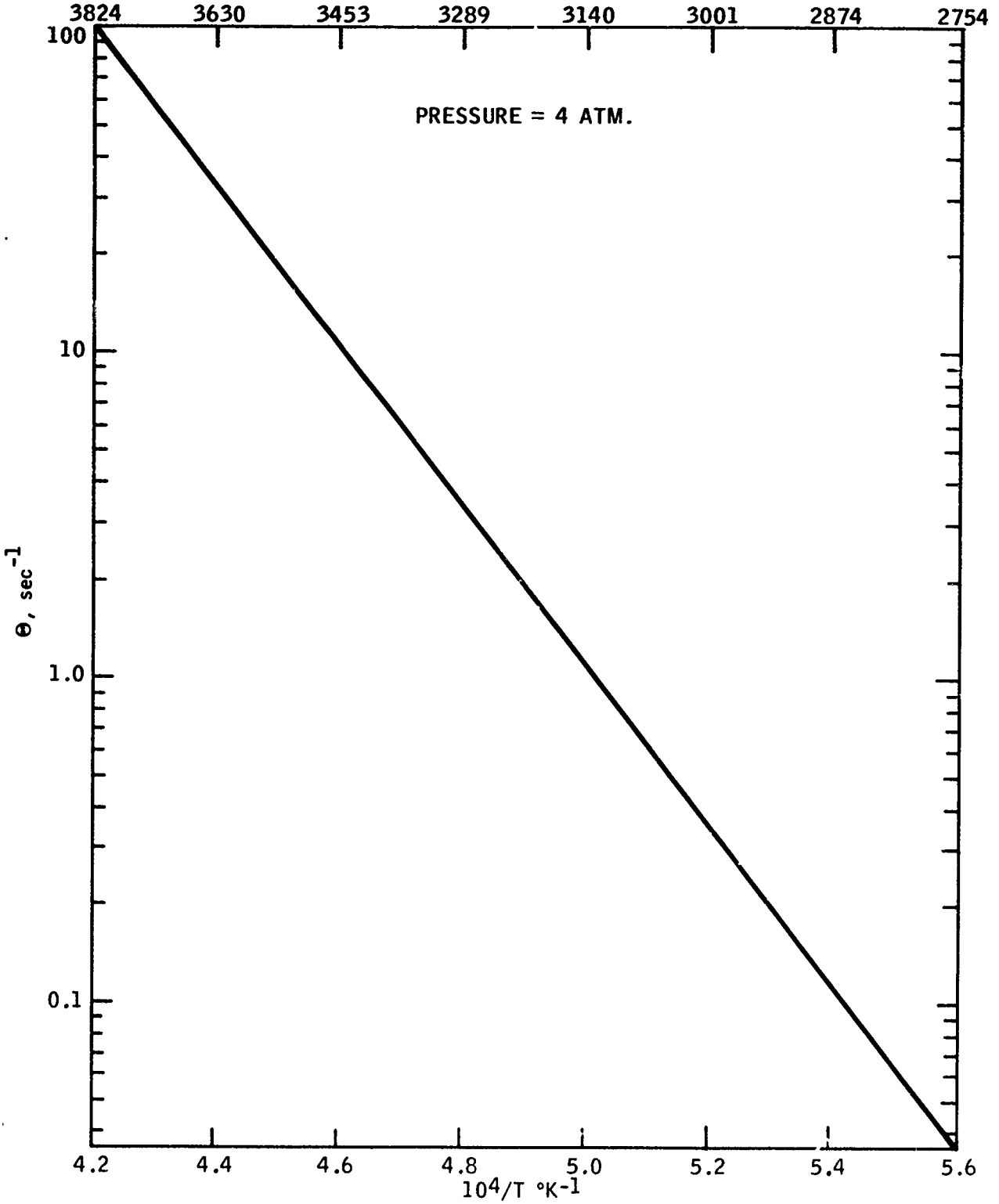

Figure 16

ARRHENIUS PLOT OF Θ

TABLE XXV

KINETIC PARAMETERS FOR EQUATION (5)

Equivalence Ratio, ϕ													Temperature	
0.8			0.9			0.95			1.0			1.1				
θ	δ	NO_x	θ	δ	NO_x	θ	δ	NO_x	θ	δ	NO_x	θ	δ	NO_x	°F	°K
			111	0.722	6014				110	0.654	3372	109	0.455	1328	3860	2400
			40.8	0.774	4830				40.6	0.709	2317	40.2	0.434	652	3680	2300
			13.7	0.821	3853				13.6	0.774	1527	13.5	0.393	286	3500	2200
			4.10	0.850	3037				4.09	0.851	963	4.04	0.345	113	3320	2100
			1.09	0.854	2350				1.09	0.942	577	1.08	0.296	40.3	3140	2000
			0.253	0.825	1774				0.252	1.05	326	0.249	0.249	12.8	2960	1900
			0.0493	0.763	1298				0.0492	1.19	173	0.0486	0.247	3.58	2780	1800
					Adiabatic Flame Temperature											
8.78	0.752	5010													3432	2162
			39.8	0.774	4830										3680	2300
						69.1	0.773	4190							3774	2352
									98.3	0.661	3230				3838	2388
												98.4	0.460	1230	3840	2389

TABLE XXVI

COMPARISON OF CALCULATED AND OBSERVED NO_x LEVELS - ADIABATIC FLAME TEMPERATURE

ϕp Apparent	ϕo Overall	Primary Zone Time sec	ρ	Distance in Can L/D	(NO_x) calc. ppm	(NO_x) obs. ppm
0.9	.27	1.5×10^{-3}	0.15	0.50	73	70
1.0	.30	1.7×10^{-3}	0.17	0.57	82	80
1.1	.33	1.9×10^{-3}	0.19	0.63	92	91

The agreement between theory and experiment is exceptionally good. The essence of the calculation is that the product Θt is proportional to the fraction of equilibrium achieved. The adiabatic flame temperature is not achieved experimentally. Thus Θ is smaller than calculated and in turn time must be longer. For example, if one assumes the primary temperature is T = 3680°F (2300°K) which is about 160°F lower than the adiabatic flame temperature, then the corresponding Θ is 40 and $(NO)_e$ = 2317. Thus lowering the flame temperature by 160°F would require an increase in residence time by almost a factor of 4 to achieve the same NO_x levels. This is illustrated in Table XXVII.

TABLE XXVII

EFFECT OF NON-ADIABATIC FLAME TEMPERATURE ON RESIDENCE TIME

ϕp Apparent	ϕo Overall	ρ	t sec	Distance in Can L/D	(NO_x) calc. ppm	(NO_x) obs. ppm
0.9	.27	0.11	5.3×10^{-3}	1.7	74	70
1.0	.30	0.12	5.9×10^{-3}	1.9	82	80
1.1	.33	0.13	6.5×10^{-3}	2.1	90	91

where, $t = 1.54 \times 10^{-3} \frac{\text{sec}}{\text{inch}}$ at 3680°F and overall L/D = 3.

APPENDIX VII

COMPUTER PROGRAM

A listing of the Fortran 4 computer program that was used to calculate the results in Appendix I, II and III is included here. The experimental results were corrected and introduced on a wet basis. The program then calculated the material balance and printed an additional set of cards containing the material balance values. The complete set of cards was then read-in to calculate the reference emissions and the effectiveness of the modifications.

```
C      PCAR= PERCENT CARBON
C      PO = PERCENT OXYGEN
       REAL NOX,NO2
       DIMENSION PHI(190),CO2(190),CO(190),HC(190),NOX(190),NO2(190),
      1TE(190),TP(190),                    PO(190),RUN(190),FUMOD( 8,190),
      2PCAR(190),P(190),O2(190)
       DIMENSION IRUN(190),ICO(190),IHC(190),IOX(190),IO2(190),ITE(190),
      1ITP(190),NUMB(190)
       DATA IN,KO/2,3/
       DO 5 I=1,184
       READ(IN,10)RUN(I),(FUMOD(II,I),II=1,8), PHI(I),CO2(I),O2(I),CO(I),
      1HC(I),NOX(I),NO2(I),TE(I),TP(I),P(I)
   10 FORMAT (F5.0, 8A4,F5.3,2F5.2,F5.0/5(F5.0),F5.1)
       PCAR(I)= ((CO2(I)+( 1.E-04*CO(I))+( 1.E-04*HC(I)))*
      1((1.89*PHI(I))+28.04)/(4.*PHI(I)))
       IF(PHI(I))3,3,2
    2  IF(CO2(I))3,3,6
    6  IF(CO(I))3,3,8
    8  IF(HC(I)) 3,3,22
    3  PCAR(I)=-PCAR(I)
   22  PO(I)=((O2(I)+CO2(I))+(5.E-05*CO(I))+( 1.E-04*NO2(I))
      1+(5.E-05* (NOX(I)-NO2(I))))*((0.321*PHI(I)) +4.76)+( 32.1*PHI(I))
       IF(PHI(I))7,7,23
   23  IF(CO2(I))7,7,25
   25  IF(O2(I))7,7,27
   27  IF(CO(I))7,7,31
   31  IF(NOX(I))7,7,33
   33  IF(NO2(I))7,7,5
    7  PO(I)=-PO(I)
    5  CONTINUE
       ICOUN=0
       IFIRS=1
       LAST=24
   13  WRITE(KO,14)
   14  FORMAT('1')
       WRITE(KO,114)
  114  FORMAT(44X,'EXPERIMENTAL RESULTS (WET BASIS)'/)
       WRITE(KO,15)
   15  FORMAT( 1X,'RUN',6X,'FUEL MODIFICATION',7X,'PHI',4X,'CO2',4X,'O2',
      14X,'CO',5X,'HC',4X,'NOX',3X,'NO2',5X,'TE',7X,'TP',5X,'P',6X,
      2'C BAL',4X,'O BAL')
       WRITE(KO,115)
  115  FORMAT(41X,'PCT',3X,'PCT',4X,'PPM',4X,'PPM',3X,'PPM',3X,'PPM',5X,
      1'F',8X,'F',5X,'PSIG',5X,'PCT',6X,'PCT'//)
       DO 200 K=IFIRS,LAST
       IRUN(K)=IFIX(RUN(K)+.1)
       ICO(K)=IFIX(CO(K)+.1)
       IHC(K)=IFIX(HC(K)+.1)
       IOX(K)=IFIX(NOX(K)+.1)
       IO2(K)=IFIX(NO2(K)+.1)
       ITE(K)=IFIX(TE(K)+.1)
       ITP(K)=IFIX(TP(K)+.1)
  200  CONTINUE
       DO 40 J=IFIRS,LAST
       WRITE(KO,30) IRUN(J),(FUMOD(JJ,J),JJ=1, 6),PHI(J),CO2(J),O2(J),
      1ICO(J),IHC(J),IOX(J),IO2(J),ITE(J),ITP(J), P(J),PCAR(J),PO(J)
   30  FORMAT(1X,I3,3X,6A4,2X,F5.3,2X,F6.2,2X,F5.1,1X,I6,2X,I3,2X,I4,3X,
      1I3,3X,I4,3X,I6,1X,F6.1,3X,F6.1,3X,F6.1/)
```

```
 40 CONTINUE
    ICOUN=ICOUN+1
    IF(ICOUN.EQ.8) GO TO 995
998 IF(ICOUN-7)45,46,46
 45 IFIRS=IFIRS+24
    LAST=LAST+24
    GO TO 13
 46 IFIRS=IFIRS+24
    LAST=LAST+16
    GO TO 13
995 NUMB(1)=0
    READ (IN,990)
990 FORMAT(1A1)
    DO 290 L=1,184
    NUMB(L)=NUMB(1)+1
    IF(PCAR(L))292,999,293
292 PCAR(L)=PCAR(L)*(-1.)
293 PCAR(L)=PCAR(L)
    IF(PO(L))294,999,295
294 PO(L)=PO(L)*(-1.)
295 PO(L)=PO(L)
    WRITE(IN,300) PCAR(L),PO(L),NUMB(L)
300 FORMAT(2(3X,F6.1),59X,I3)
    NUMB(1)=NUMB(L)
290 CONTINUE
999 CALL EXIT
    END
```

```
C  PCT CO AND PCT O REFERENCE   -   PCT CHANGE CO AND PCT CHANGE O
C     PCARR = PER CENT CARBON  (REFERENCE)
C     POR = PER CENT OXYGEN    (REFERENCE)
C     CPAR = PCT CHANGE (CO)
C     CPO = PCT CHANGE (O)
      REAL NOX,NO2,NOXR,NO2R,NNOX,NNO2
      DIMENSION CO2R(190),O2R(190),COR(190),HCR(190),NOXR(190),
     1NO2R(190), TER(190),TPR(190),PCARR(190),POR(190),ICOR(190),
     2IHCR(190),INXR(190),IO2R(190),ITER(190),ITPR(190)
      DIMENSION PHI(190),CO2(190),CO(190),HC(190),NOX(190),NO2(190),
     1TE(190),TP(190),IRUN(190),P(190),O2(190),RUN(190),FUMOD( 8,190)
      DIMENSION CCO2(190),CHO2(190),CCO(190),CHC(190),NNOX(190),
     1NNO2(190),CTE(190),CTP(190),CPCAR(190),CPO(190)
      DIMENSION ICCO(190),ICHC(190),INOX(190),INO2(190),NITER(190),
     1NITP(190),PCAR(190),PO(190)
      DATA IN,KO/5,6/
      DO 5 I=1,184
      READ(IN,10)RUN(I),(FUMOD(II,I),II=1,8), PHI(I),CO2(I),O2(I),CO(I),
     1HC(I),NOX(I),NO2(I),TE(I),TP(I),P(I),PCAR(I),PO(I)
   10 FORMAT (F5.0, 8A4,F5.3,2F5.2,F5.0/5(F5.0),F5.1/2(3X,F6.1))
    5 CONTINUE
      DO 100 L=1,46
      CO2R(L)=12.162*PHI(L)
      O2R(L)=20.059*(1.0-PHI(L))
      COR(L)=(-11919.*PHI(L))+6404.6053
      HCR(L)=(1812.9*PHI(L))-508.47181
      IF(HCR(L))400,400,401
  400 HCR(L)=0.0
  401 NOXR(L)=(185.74*PHI(L))+29.624074
      NO2R(L)=(55.772*PHI(L))-2.239382
      TER(L)=(2461.0*PHI(L))+768.04131
      TPR(L)=(2373.4*PHI(L))+807.89877
      PCARR(L) = ((CO2R(L)+(1.E-04*COR(L))+(1.E-04*HCR(L)))*
     1((1.89*PHI(L))+28.04)/(4.*PHI(L)))
   22 POR(L) = ((O2R(L)+CO2R(L))+(5.E-05*COR(L))+( 1.E-04*NO2R(L))
     1+(5.E-05*(NOXR(L)-NO2R(L))))*((0.321*PHI(L)) + 4.76)
     2+(32.1*PHI(L))
  100 CONTINUE
      DO 105 M=47,184
      CO2R(M)=12.189*PHI(M)
      O2R(M)=20.751*(1.0-PHI(M))
      COR(M)=(-47141.*PHI(M))+18051.82
      HCR(M)=(-722.12*PHI(M))+86.48685
      IF(HCR(M))402,402,403
  402 HCR(M)=0.0
  403 NOXR(M)=(343.59*PHI(M))-22.953053
      NO2R(M)=(178.38*PHI(M))-34.078409
      TER(M)=(3350.9*PHI(M))+516.24596
      TPR(M)=(3088.2*PHI(M))+596.69639
      PCARR(M) = ((CO2R(M)+(1.E-04*COR(M))+(1.E-04*HCR(M)))*
     1((1.89*PHI(M))+28.04)/(4.*PHI(M)))
  220 POR(M) = ((O2R(M)+CO2R(M))+(5.E-05*COR(M))+( 1.E-04*NO2R(M))
     1+(5.E-05*(NOXR(M)-NO2R(M))))*((0.321*PHI(M)) + 4.76)
     2+(32.1*PHI(M))
  105 CONTINUE
      ICOUN=0
      IFIRS=1
      LAST=24
```

```
 13 WRITE(KO,14)
 14 FORMAT('1')
    WRITE(KO,184)
184 FORMAT(44X,'REFERENCE EMISSIONS (WET BASIS)'/)
    WRITE(KO,15)
 15 FORMAT( 1X,'RUN',6X,'FUEL MODIFICATION',7X,'PHI',4X,'CO2',5X,'O2',
   14X,'CO',4X,'HC',4X,'NOX',3X,'NO2',6X,'TE',8X,'TP',5X,'P',6X,
   2'C BAL',4X,'O BAL')
    WRITE(KO,115)
115 FORMAT(41X,'PCT',4X,'PCT',4X,'PPM',3X,'PPM',3X,'PPM',3X,'PPM',6X,
   1'F',9X,'F',4X,'PSIG',6X,'PCT',6X,'PCT'//)
    DO 200 K=IFIRS,LAST
    IRUN(K)=IFIX(RUN(K)+.1)
    ICOR(K)=IFIX(COR(K)+.1)
    IHCR(K)=IFIX(HCR(K)+.1)
    IOXR(K)=IFIX(NOXR(K)+.1)
    IO2R(K)=IFIX(NO2R(K)+.1)
    ITER(K)=IFIX(TER(K)+.1)
    ITPR(K)=IFIX(TPR(K)+.1)
200 CONTINUE
    DO 40 J=IFIRS,LAST
    WRITE(KO,30) IRUN(J),(FUYOD(JJ,J),JJ=1, 6),PHI(J),CO2R(J),O2R(J),
   1ICOR(J),IHCR(J),IOXR(J),IO2R(J),ITER(J),ITPR(J),P(J),PCARR(J),
   2POR(J)
 30 FORMAT(1X,I3,1X,6A4,2X,F5.3,1X,F6.2,1X,F6.1,1X,I6,2X,I3,2X,I4,3X,
   1I3,3X,I6,3X,I6,1X,F6.1,3X,F6.1,3X,F6.1/)
 40 CONTINUE
    ICOUN=ICOUN+1
    IF(ICOUN.EQ.9) GO TO 997
998 IF(ICOUN-7)45,46,46
 45 IFIRS=IFIRS+24
    LAST=LAST+24
    GO TO 13
 46 IFIRS=IFIRS+24
    LAST=LAST+16
    GO TO 13
997 DO 300 N=1,184
    CCO2(N) = ((CO2(N)-CO2R(N))/ CO2R(N))*100.
    CHO2(N) = ((O2(N)-O2R(N))/ O2R(N))*100.
    CCO(N) = ((CO(N)-COR(N)) / COR(N))*100.
    IF(HCR(N))999,991,992
991 CHC(N)=0.0
    GO TO 993
992 CHC(N) = ((HC(N)-HCR(N)) /HCR(N)) *100.
993 CNOX(N) = ((NOX(N)-NOXR(N)) /NOXR(N))*100.
    CNO2(N) = ((NO2(N) -NO2R(N)) / NO2R(N))*100.
    CTE(N) = ((TE(N)-TER(N))/ TER(N))*100.
    CTP(N) = ((TP(N)-TPR(N)) / TPR(N))*100.
    CPCAR(N)= ((PCAR(N)-PCARR(N))/PCARR(N))*100.
 52 CPO(N) = ((PO(N)-POR(N))/POR(N))*100.
300 CONTINUE
    ICOUN=0
    IFIRS=1
    LAST=24
 93 WRITE(KO,94)
 94 FORMAT('1')
    WRITE(KO,194)
194 FORMAT(44X,'PER CENT CHANGE DUE TO MODIFICATION'/)
```

```
      WRITE(KO,95)
   95 FORMAT( 1X,'RUN',6X,'FUEL MODIFICATION',7X,'PHI',4X,'CO2',5X,'O2',
     14X,'CO',5X,'HC',7X,'NOX',5X,'NO2',6X,'TE',5X,'TP',5X,
     2'C BAL',3X,'O BAL')
      WRITE(KO,915)
  915 FORMAT(41X,'PCT',5X,'PCT',3X,'PPM',4X,'PPM',6X,'PPM',5X,'PPM',6X,
     1'F',6X,'F',7X,'PCT',5X,'PCT'//)
      DO 500 LI=IFIRS,LAST
      IRUN(LI)=IFIX(RUN(LI)+.1)
      WRITE(KO,70) IRUN(LI),(FUMOD(LL,LI),LL=1,6),PHI(LI),CCO2(LI),
     1CHO2(LI), CCO(LI), CHC(LI),NNOX(LI),NNO2(LI),CTE(LI),CTP(LI)
     2,      CPCAR(LI),CPO(LI)
   70 FORMAT(1X,I3,3X,6A4,2X,F5.3,1X,F6.2,1X,F6.2,1X,F6.2,2X,F6.2,2X,
     1F6.2,2X,F6.2,2X,F6.2,2X,F6.2,2X,F6.2,2X,F6.2,2X,F6.2//)
  500 CONTINUE
      ICOUN=ICOUN+1
      IF(ICOUN.EQ.8) GO TO 999
  996 IF(ICOUN-6)74,74,64
   74 IFIRS=IFIRS+24
      LAST=LAST+24
      GO TO 93
   64 IFIRS=IFIRS+24
      LAST=LAST+16
      GO TO 93
  999 CALL EXIT
      END
```